

Advanced Vehicle Power Technology Alliance Fiscal Year 2016 (FY16) Annual Report (1 Oct 2015 – 30 Sep 2016)

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(RDTA-COS)
Department of Energy



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ACKNOWLEDGEMENTS

The Advanced Vehicle Power Technology Alliance (AVPTA) between the Department of Energy (DOE) and the Department of the Army (DA) was publicly announced in July 2011. The Alliance underscores the urgency for energy security; in particular, an emphasis on developing advanced technologies that enable military ground vehicles to become significantly more energy efficient. Individually and collaboratively, the DOE and DA have a long history of successfully developing innovative vehicle technologies. The Alliance is chartered to accelerate the conceptualization and transition into deployment of inventive and creative energy-saving concepts that the Nation needs to achieve energy security.

This report summarizes the fifth year of technical effort and output of the Alliance's Technology Focus Area (TFA) working groups that were established in July 2011. The TFAs are respectively led by DOE and DA Subject Matter Experts (SMEs) that jointly recommend and oversee project portfolios in areas of interagency mutual technical interest.

We acknowledge the significant contributions of the DOE and DA administrative and technical personnel who in five years have grown the Alliance from a notional concept into a self-sustaining and highly-productive entity. Work product generated by the Alliance has migrated into commercial and military applications through industry partners. In parallel with ongoing activities, DOE and DA personnel have extended the AVPTA enterprise into new areas of engagement including the Office of the Secretary of Defense Operational Energy Plans and Programs (OSD/OEPP)-sponsored "Increasing the Fuel Efficiency of the Current Ground Tactical Fleet" (IFECGTF) Program; the project portfolio of which includes autonomy-enabled, vehicle electrification and powertrain technology-related activities.

We specifically acknowledge Ms. Katherine Hammack, who as Assistant Secretary of the Army for Installations, Energy & Environment provided invaluable insight and direction to the Alliance from its inception through to and including her final status/update briefing in December 2016. We also acknowledge Mr. David Howell and Ms. Christy Cooper, who as DOE-VTO Acting Directors, seamlessly supported the Alliance through VTO's leadership transition.

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EXECUTIVE SUMMARY

The AVPTA Mission is to leverage “resources to improve transition of technologies into both the commercial and military marketplace,” and “industrial research and development (IRAD) involving commercial automotive and defense ground vehicle manufacturers to transition technologies and increase precompetitive research and development.”

The following summaries document the work product of thirty (30) projects contained within the AVPTA portfolio. Project performers include Automotive Industry Original Equipment Manufacturers (OEMs) and Tier 1 / 2 Suppliers, Defense Industry OEMs and Suppliers, DOE National Laboratories, DOD Research Laboratories, Contract Research Organizations, Universities and Colleges, Small and Other Category Businesses.

Some of the projects reported upon herein were among the seven (7) original projects that formed the Alliance’s foundation and enabled its rapid start-up. In many instances, DOE and DA mutually leveraged respective ongoing projects by infusing personnel, contributing resources, and providing mutual experience/expertise. This quickly expanded the Alliance technical network and reach, and provided access to activities beyond those directly funded by the Alliance. An example is TARDEC SME engagement in the VTO Annual Merit Review (AMR) during which TARDEC personnel are exposed to the complete VTO project portfolio including participating/contributing as review panel members. Joint participation in the AMR helps to formulate areas of mutual technical interest (AOIs) that contain the description, scope and deliverables for future new-start projects.

Also reported upon herein are projects that were jointly selected for start-up in Fiscal Years 14, 15 & 16. The Alliance has developed and instituted a sustainable, new-start project review and selection process based upon VTOs annual Funding Opportunities Announcements process and timeline. The process leverages DOE’s National Energy Technology Laboratory Contract Office to rapidly obligate and efficiently track project funding by individual performer.

Through FY16, DOE and DA have jointly contributed to the Alliance funds totaling \$142.6M. The result has been a level of effort/output that neither agency would have realized without the interagency collaboration.

Among her closing comments during the December 2016 status/updates briefing, Ms. Hammack commented that AVPTA has far exceeded all expectations for technical performance and has become the reference model for interagency collaboration. The Alliance is the prototype after which the OSD/OEPP-sponsored IFECGTF and JP-8 Fuel Cell Power Programs are structured.

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INTRODUCTION

There are two high level drivers that led to the development of the AVPTA. The first is the elevation of energy efficiency and security as points of emphasis throughout the Army and the Department of Defense (DOD) as a whole. For the Army, a major milestone in this was the development of the Army Energy Security Implementation Plan (AESIP) in 2009. Within the AESIP goal to Increase Energy Efficiency across Platforms and Facilities, there was an objective to increase the efficiency of tactical equipment. At the DOD level, the Operational Energy Strategy is a principle-guidance document for the Department's approach to ensure energy security for operational forces.

The second was a call by the DOD for strengthened interagency partnering. This was set forth in its 2010 Quadrennial Defense Review. Energy security was identified as an excellent opportunity area for such a partnership. To this end, the DOE and DOD worked to craft a Memorandum of Understanding (MOU) to establish a partnering framework to enhance national energy security. This MOU is included as Appendix A. The MOU calls for the Departments to work together in a wide range of technical areas; including efficient transportation and overall energy efficiency.

DA and DOE worked together under the auspices of this MOU to develop a charter for working together in a wide range of vehicle technologies. This charter describing the Alliance was originally signed by the Honorable Daniel B. Poneman, Deputy Secretary of Energy and the Honorable Joseph W. Westphal, Under Secretary of the Army; and in 2016 was renewed/extended for five (5) additional years under the signatures of the Honorable Elizabeth Sherwood-Randall, Deputy Secretary of Energy and Honorable Patrick J. Murphy, Under Secretary of the Army (see Appendix B).

The DOE mission is to ensure America's security and prosperity by addressing its energy, environmental, and nuclear challenges through transformative science and technology solutions. A critical step in any new technology development is having it accepted and deployed in the marketplace. Teaming with DOD provides an attractive pathway for early utilization of the novel energy-saving ideas coming from the DOE research portfolio. These agencies strategic goals are summarized in the following table:

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DOD & DOE Strategic Goals

DOD Operational Energy Strategy	DOE Vehicle Technologies Office
Reduce Energy Demand: - Reduce: • Overall Operational Energy Demand • Mission Risks & Costs - Improve Energy Usage Efficiency	Improve Energy Efficiency of the Transportation Sector
Expand & Secure Energy Supply: - Diversify Energy Sources - Protect Energy Supply Access	Increase Domestic Energy Security Reduce Petroleum Consumption Reduce Operating Cost for Consumers and Business
Integrate Operational Energy Considerations Into: - Planning Activities and Force Development	Improve Global Competitiveness of U.S. Industry Improve Domestic Manufacturing

With strong support from senior leadership, the agencies collaborated at the Executive and SME Levels to identify AOIs that are the founding principles for describing each of the Alliance's Technology Focus Areas (TFAs). The respective TFA descriptions follow.

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TECHNOLOGY FOCUS AREA (TFA) DESCRIPTIONS

TFA1: Advanced Combustion Engines & Transmissions

Advanced air-fuel management systems and novel combustion regimes have the potential to dramatically increase efficiency and power density, while at the same time reducing emissions. Meeting the challenge of developing and optimizing the combustion of common petroleum fuels, including Jet Propellant-8 (JP8), or biofuels in advanced engines requires a new level of the understanding of the physical and chemical phenomena of the Direct Injection (DI) diesel engine, which will be strongly affected by the different fuel properties which in turn affect fuel/air mixture preparation, combustion and emissions.

Advanced transmissions can allow the engine to operate more frequently in regions of high efficiency and transmit more torque while maintaining drivability. Of particular interest for further Research & Development (R&D) are approaches and devices to increase launch-assist device efficiency, and to increase the number of gear ratios. Among possible options for investigation are higher gear count automatic transmissions, Dual Clutch Transmissions (DCT), wet and dry clutch launch devices, multi damper torque converters, Continuously Variable Transmissions (CVTs), and binary transmissions.

TFA2: Lightweight Structures & Materials

Reduction of vehicle gross weight is an effective approach to reduce energy consumption during the vehicle usage, regardless of their energy sources (e.g., liquid fuels or electric batteries). Lightweight materials such as aluminum (Al) alloys, magnesium (Mg) alloys, high-strength steel, and carbon-polymer composites have been considered to replace low carbon steels conventionally used in automotive components. Challenges exist, however, to integrate components made of these lightweight materials into vehicle structures to achieve maximum weight reduction, while maintaining structural rigidity, crash safety, production quality and cost parity.

TFA3: Energy Recovery & Thermal Management

In current vehicles, approximately 60% of the chemical energy of fuel is lost in the form of waste heat, dissipated by the exhaust and cooling systems. The former offers high-grade heat that approaches temperatures of 800°C while the latter is a considerably more modest heat source at approximately 120°C. Of significant interest are exhaust heat recovery systems, including Organic Rankine cycles, as well as mechanical and electrical turbo-compounding. In addition, through the development of cost-competitive advanced second generation thermoelectric (TE) devices for vehicle applications vehicle fuel efficiency, performance, and emissions can be improved. Thermo-electric devices can convert engine waste heat to useful electrical power, to be used either assisting propulsion or for powering hotel loads. By integrating high Figure of Merit TE devices in the vehicle architecture, thermal management of vehicles can become significantly more efficient.

TFA4: Alternative Fuels & Lubricants

Alternative fuels and lubricants can facilitate or enhance conventional engine technology, as well as advanced combustion regime engine operation such as Homogeneous Charge Compression Ignition (HCCI) or Low Temperature Combustion. For alternative fuels, the focus should be on drop-in fuels or blend stocks that displace petroleum-derived fuels in vehicle applications without significant infrastructure changes or requirements. New developments in base oil and additive packages can reduce viscosity while maintaining temperature requirements, thereby improving engine and transmission efficiency.

TFA5: Electrified Propulsion Systems

Electric drive options range from mild battery-alternator systems to full parallel and series systems or all electric drive, and require engineering trade-offs between fuel consumption benefit and system complexity, reliability and cost. However, to achieve efficient solutions, electrical materials and devices will require higher conversion efficiencies and power/energy densities than are currently possible. The next generation electric drive vehicles will benefit from improved and lower cost batteries, novel electric motors, thermoelectric waste heat recovery, and power electronic devices and electrical topologies that are capable of handling increased loads and multiple combinations of sources and accessories. Activities focus on hybrid system power electronics and electric machines.

TFA6: Energy Storage & Batteries

Stakeholders desire to improve existing battery chemistries, develop advanced battery technologies (high power and high energy systems), and conduct ultra-capacitor research. Military goals are to improve the availability of onboard power, reduce energy demand/consumption, expand the energy supply to military operations and build energy security into future forces in the specific areas of: silent watch capability, electromagnetic armor and starting/lighting/igniting (SLI). Civilian/commercial goals are to reduce the petroleum demand and promote US economic competitiveness in advanced hybrid electric vehicles and electric vehicles. Advanced lead-acid batteries, ultra-capacitors, lithium-ion batteries, lithium sulfur and lithium-air batteries are joint areas of interest. Both agencies are also interested in improving on-board safety, developing battery test protocols and promoting codes and standards.

TFA7: Analytical Tools (Modeling & Simulation)

Diverse fuel sources, advanced combustion modes, hybrid/electrified powertrains, energy harvest/waste heat recovery technologies, and using lightweight materials substantially elevate the complexities of efficient vehicle powertrain systems and impose critical challenges for system integration and control. These efficient vehicle powertrain sub-systems, with new characteristics and strongly interactive dynamics, necessitate research on system integration and advanced control strategies. An integrated and analytical systems approach ensure that the various sub-systems of the vehicle work seamlessly, reliably and synergistically to optimize coordination so as to maximize vehicle energy efficiency, power density and emission reduction potential in real-world

applications. Through state-of-the-art modeling and analysis, concepts and strategies can be screened during the vehicle design stage, and most promising candidates and key pathways to bring them to realization in an effective time frame can be identified. Critical components and/or systems needing specific development can also be identified and analyzed with simulation tools.

TFA9: Autonomy-enabled Technologies

Autonomy-enabled technologies have the promise to significantly decrease fuel consumption through a variety of mechanisms. For example, platooning, where vehicles travel close to each other in order to reduce aerodynamic drag at high speeds, can only be achieved through connectivity and automation. A significant source of excess fuel consumption comes from vehicle operators driving in a sub-optimal manner, such as exceeding optimal speeds and accelerating and decelerating too quickly. Intelligent systems can help increase fuel efficiency by providing information to the driver to improve operational behavior, by determining more efficient routes based on topography or traffic conditions, or by taking control of certain vehicle functions. An automated traffic management system, implemented through a system of autonomous vehicles connected with intelligent roadway infrastructure, could greatly reduce vehicle start/stops and slowdowns, optimizing traffic flow, and improving mobility in urban driving. Preliminary research by the National Renewable Energy Laboratory (NREL) indicates that platooning could increase fuel efficiency by 10%, eliminating driver inefficiencies another 15%, and completely automating the vehicle transportation system could yield a 40% improvement. However, these estimates are based on a limited number of experiments, which may not include the full range of variability that a real world system would experience, nor potential second-order effects, such as an increase in vehicle miles traveled. Accordingly, additional analysis and targeted experimentation are needed to more fully explore the limitations that these autonomy-enabled technologies may have in regards to increasing fuel efficiency across the transportation system.

PROJECT TECHNICAL REPORTS

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AVPTA Technology Focus Area 1: Advanced Combustion, Engines & Transmissions

DOE-VTO TFA Lead: Gurpreet Singh
TARDEC TFA Lead: Dr. Peter Schihl

There was no project activity under this TFA during FY16.

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AVPTA Technology Focus Area 2: Lightweight Materials and Structures

Light Weight Vehicle Structure (LWVS)

DOE-VTO TFA Lead: Sarah Ollila
TARDEC TFA Lead: Martin McDonnell

Principal Investigator:
Dr. Richard Gerth

Affiliation: TARDEC
Product Lifecycle Engineering - Materials

Project Start: Q1FY13
Estimated Completion: Q3FY17

Objective(s):

- Design, manufacture, and evaluate lightweight, multi-material military vehicle structure that is both affordable and 30% lighter weight.
- Evaluate commercial defense barriers to lightweight material technology adoption.

Strategic Context:

- Evaluation structure is the LAV-25 turret. Technologies and lessons learned may be transferable to new turrets, such as Combat Vehicle Prototype (CVP), Next Generation Combat Vehicle (NGCV), and Future Fighting Vehicle (FFV).
- The turret is a multi-material turret, which is a technology explicitly mentioned in the Lightweight Combat Vehicle Science and Technology Campaign (LCVSTC)
- The turret will provide insight to guide future R&D directions necessary to overcome barriers to adoption of the light-weighting technologies.

Accomplishments:

- Gun Fire Testing successfully completed
- Ballistic impact evaluation successfully completed
- Cold and hot weather storage testing successfully completed
- Lifting test successfully completed
- Results presented and published at NATO meeting

Introduction:

Vehicle lightweighting is a priority for the US. Army (Polson, et al., Lightweight Combat Vehicle Science and Technology Campaign, 2014). The future force must be more expeditionary and agile to the ever changing global threat environment. Due to increased survivability requirements, additional protection measures have been added to vehicles, which has typically increased their weight. The increased weight has resulted in decreased fuel economy, decreased reliability and associated vehicle availability, and in some cases, decreased swim, fording, and transport capability. Further, as vehicle weight increases through the Engineering Change Proposal (ECP) process, operational capability may degrade [2].

A true multi-material structure for a military vehicle has not yet been produced for production. The FCS ARES was a hybrid monocoque / space frame architecture that was predominantly aluminum and composites (Pike & Filar, 2009). It was a multi-material structure which demonstrated the state of the art. The LWVS program is not designed to show the state of the technical art, but rather the state of the commercial art. In other words, it is not a study in how much weight can technically be eliminated through material optimization, but rather how much weight can be eliminated from a current military vehicle using commercially available and affordable technologies. The project tests the hypothesis that multi-material technologies developed for the commercial automotive industry can be adapted for military applications to significantly reduce vehicle weight for an acceptable cost. The ultimate goal of the project, if successful, is to transition the adapted technologies into a current military vehicle through a future upgrade program.

Approach:

The LWVS program is not designed to show the state of the technical art, but rather the state of the commercial art. In other words, it is not a study in how much weight can technically be eliminated through material optimization, but rather how much weight can be eliminated from a current military vehicle using commercially available and affordable technologies. The project tests the hypothesis that multi-material technologies developed for the commercial automotive industry can be adapted for military applications to significantly reduce vehicle weight for an acceptable cost. The ultimate goal of the project, if successful, is to transition the adapted technologies into a current military vehicle through a future upgrade program.

The demonstration platform for the LWVS is the Marine Light Armored Vehicle (LAV-25). The LWVS program is a multi-year program structured in three phases (see Figure 3):

1. Trade Study and Technology Development (14 months)
2. Detailed Design and Manufacture (18 months)
3. Test and Evaluation (12 months).

Program results for Phase I, Phase II, and limited Phase III results have been published in prior year AVPTA reports (Davis & Rogers, Advanced Vehicle Power Technology Alliance Fiscal Year 2014 Annual Report, 2015) [4], as well as several open literature publications [5] [6]. While this report focuses on the results achieved during FY2016, some of the information published previously will be repeated for context and understanding.

Results and Discussion:

The primary focus of the year has been on testing and evaluation. The specific tests that were conducted are:

1. *Gun Firing Test*
2. *Ballistic Impulse Transfer Test*
3. *Cold and Hot Weather Storage Test*
4. *Lifting Test*
5. *Cold and Hot Weather Durability Test*

Gun Firing Test

As reported previously [4] [6], turret stiffness was a major concern, as it affected gun firing accuracy during repeated fire. For this reason the baseplate was thickened and its fiber specification was changed to a high modulus 50 Msi fiber. The added thickness, fiber change, and local geometry reinforcements added 35 lbs and in azimuth and elevation stiffness values that were within 10% of the current steel design. This enabled both stabilized and power mode turret operation without changes to the gun firing software.

The turret was integrated with the vehicle, and the complete system was shipped to Aberdeen Proving Grounds. The Aberdeen Test Center conducted the tests. The 25 mm main gun, co-axial machine gun, and smoke grenade launchers were tested.

The main gun accuracy tests were conducted over several weeks in multi-round bursts at high rate of fire at two different ranges and 4 weapon/target scenarios. The scenarios are the 4 combinations of weapon and target moving or being stationary. Stationary targets were considered to be frontal engagements, and therefore smaller than moving targets, which were considered to be flank engagements. From the measurements a probability of hit was computed assuming a normal distribution on shot variation. While the specific results will not be presented here, there were no issues discovered with the accuracy of the 25 mm gun related to the composite turret integration.

The co-axial gun while also shot in repeated multi-round bursts at high rate of fire, was only tested at one range and against stationary targets while the vehicle was also stationary.

The smoke grenade launchers were also tested. Both left and right side grenade launchers were fired simultaneously to impart the maximum impulse into the turret (see Figure). This was repeated 4 times. While accuracy was not an issue, damage to the turret or other elements was not discovered during post-test inspection.

Ballistic Impulse Transfer Test

The existing steel turret structure is composed of high hard plates which contribute to the armor protection. In addition there is add-on armor to provide protection against more energetic threats. The new turret utilizes carbon fiber composite side walls, which while strong, are relatively brittle and contribute little to ballistic protection. Thus a new add-on armor package that combines the ballistic protection of the original steel turret with its add-on armor is required. An armor recipe was selected that defeats the specified threat, but it is heavier than the current add-on armor. Since armor development is outside the scope of the project, the new armor was not incorporated. Yet, it is important to understand whether the composite structure is able to withstand the ballistic shock loads transferred from the armor. The specific armor attachment mechanism was described previously [4] [6].

It was necessary to develop a surrogate armor solution that transmitted the equivalent impulse to the composite structure. The impulse transmitted is the result of the energy quantity imparted to the armor minus the energy absorbed by the armor in plastic and elastic deformation. A measure of the energy imparted to the armor is the velocity of the threat projectile. The impulse is a strong function of the armor mass. Since the amount of energy absorbed is unknown, only the velocity and mass equivalence were used to choose between alternative surrogate armor choices.

Four options of surrogate armor were analyzed (see Table 1). It should be noted that as described above, they are mass equivalent, not ballistically equivalent to the designed armor. They differ in the metallic insert within the armor matrix used to defeat the threat. Option 0 is the target armor to which the other 4 are compared. The surrogate should be as close to the target armor as possible. The table shows the mass equivalence and the relative threat speed the surrogate armor can defeat. Based on this data, option 2 was selected.

The surrogate armor was affixed to full-size sidewall components, which were made in the same manner and from the same material as the sidewall that was integrated in the vehicle turret. The sidewall-armor combination was located in a specially designed and manufactured fixture. The combination was then shot at at multiple angles of obliquity in multiple locations. None of the shots penetrated and the support system was not damaged. Specific results are still pending final analysis.

Lifting Test

A major load test is the lifting of the turret assembly from the vehicle (see Figure 2). While the weight reduction of the structure was approximately 28% [6], the turret assembly still weighed almost 5,000 lbs. The lifting eyes were redesigned, because of the redesigned steel roof and carbon fiber composite sidewalls. Further, turret stiffness under static load was also a concern, just as it was under dynamic gun firing loads.

The test method was to install 48 strain gages around the lifting eyes (see Figure 3). Of particular concern was the rear lifting eye. Because the various interfaces to existing equipment could not be changed, and due to stiffness concerns with the rear of the turret, a special composite

internal rear lift eye reinforcement bracket was developed during the turret design. A major question was how much strain this reinforcement would experience.

Prior to the lift test, the rear bustle rack, add-on turret armor, and Line Replaceable Units were removed from the turret. The turret was allowed to recover from any prior environmental temperature evaluations and lifted at ambient laboratory temperature.

The results are shown in Table 2.

As expected the rear lift eye and the rear lift eye brace experienced the most strain in the up/down and fore/aft directions. One can see how this would be given there is only 1 lifting eye in the rear and 2 in the front. All the values are considered small, and hence the lifting test was considered successful.

Cold and Hot Weather Storage Test

Cold and hot weather storage tests were conducted to determine the turret structure's overall sensitivity to temperature variation. An environmental chamber was constructed around the vehicle, and it was cooled to -40 and heated to 120. While testing is complete, detailed results are still pending.

Cold and Hot Weather Durability Test

Durability testing was conducted by placing the vehicle on shaker pedestals, one under each wheel. These pedestals are computer controlled to simulate driving the vehicle over predetermined terrains. These tests are typically conducted such that the vehicle sees the loads encountered during the life of the vehicle as measured in simulated miles travelled. Typically the test runs continuously 24 hours for 7 or more days to acquire sufficient miles.

The hot and cold testing was conducted by encasing the vehicle and the shaker pedestals inside an environmental chamber that was heated to 120 for the hot and -40 for the cold weather tests. The combination of continuous operation at the extreme temperatures represents an extreme test. The purpose of the test is to determine the turret structure's sensitivity to repeated automotive loads and shocks at these extreme temperatures. The hot test was conducted first. The cold test was conducted after the hot test was completed. The vehicle was able to stabilize its temperature while the environmental chamber was converted from hot to cold testing. Further, the durability portion of the tests did not start until the chambers reached their prescribed temperatures.

While the tests are complete, detailed results are still pending. It is known that the vehicle survived the hot testing. However during cold tests, vehicle suspension systems failed. Testing was curtailed after the second suspension system failed.

Conclusions:

The Lightweight Vehicle Structure program has already shown that a lighter weight, multi-material substructure is currently possible. The aluminum-steel monocoque turret provides the

same or better performance while reducing weight by approximately 420 lbs (28%). The major difference between this program and other previous weight savings programs is that rather than creating a structure from a single material, this project utilizes the most effective material that meets the need for each component.

Future work would have to determine whether resin composite materials are competitive from a cost and performance point of view to be utilized by a defense prime to meet light-weighting needs of a military vehicle. This would not only be a function of production cost and product performance, but also of testing and repairability cost. It is anticipated that testing and repairability costs could be a significant barrier to adoption. Therefore, any future expansion of this project would have to address the question of how to reduce the test and evaluation cost of a hypothetical upgrade program involving a composite turret to the point that testing costs are equivalent to those for a monocoque metallic turret. The testing issue is primarily an issue for upgrade programs. It would not be as much of an issue for new start programs, as they have to evaluate the complete vehicle regardless of the materials selected. Another major research component would be repair technologies, their performance, as well as training requirements and the impact on the material logistics chain.

The project has thus far demonstrate that it is possible to design and manufacture a multi-material turret that is significantly lighter and meets performance requirements. The turret structure itself was 51% lighter and with the proposed add-on armor 28% lighter than the current steel turret package. Initial performance test results are positive. Additional testing is planned and will be concluded in 2017. The affordability study will also be concluded in 2017.

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- [5] R. J. Gerth, "Trade Study of a Lightweight, Multi-Material Military Vehicle Structure," in *2013 NDIA Ground Vehicle Systems Engineering and Technology Symposium, 21-22 August 2013.*, Troy, MI, 2013.
- [6] R. J. Gerth, "A Lightweight, Multi-Material Turret Structure," in *NATO AVT-264/RSM-043 Specialist's Meeting on Design, Manufacturing and Application Of Metallic Lightweight Material Components For Military Vehicles*, Tallinn, Estonia, 2016.

Figures and Tables:



Figure 1. Instrumented LAV25 Firing Smoke Grenades



Figure 2. Lift Fixture Attached to the Multi-Material Turret.

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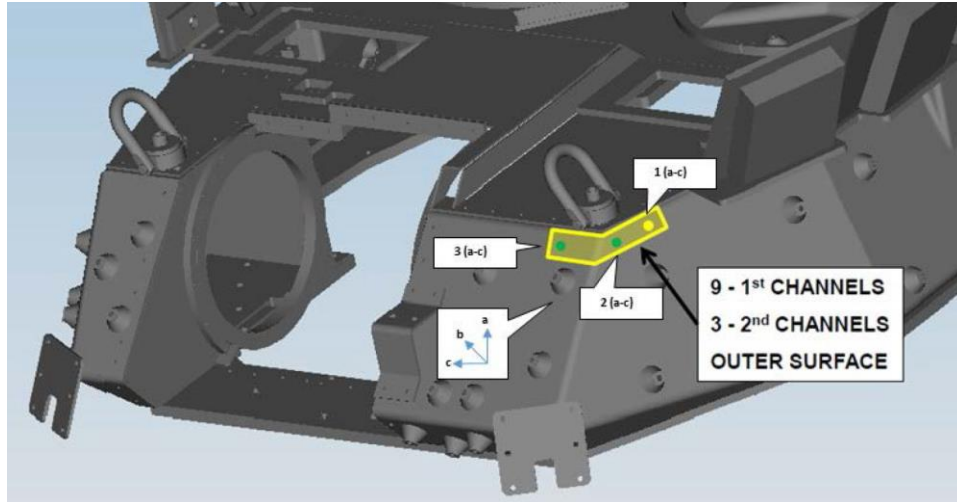


Figure 3. Example Placement of Strain Gages for Front Left Lifting Eye.

Option	Front Plate	Total Areal Density (psf)	Relative Threat Speed
0	Intended Lightweight Armor	100%	100%
1	A" 6061-T651 Aluminum	92%	100%
2	B" 6061-T651 Aluminum	101%	108%
3	C" RHA Steel, Class 1	101%	82%
4	D" RHA Steel, Class 1	141%	100%

Table 1. Comparison of 4 Alternative Surrogate Armors [4].

Location	Max	Min
Left Eye	11	-74
Right Eye	101	-20
Rear Eye Brace	281	-27
Rear Eye	30	-621

Table 2. Summary Statistics for Microstrain Values for Turret Lift Test.

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AVPTA Technology Focus Area 2: Lightweight Structures & Materials

Multi-Material Joining (MMJ) - Thermal Friction Stir Welding

DOE-VTO TFA Lead: Sarah Ollila
TARDEC TFA Lead: Martin McDonnell

Principal Investigator:
Mr. Eugene Creed

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Project Start: Q2FY15
Estimated Completion: Q3FY17

Objective(s):

- Develop a production-representative manufacturing process to join high hardness armor steel with AA6061 aluminum alloy using a bimetallic friction stir welding (FSW) process.
- Demonstrate technical feasibility by producing up to 36-inch long weld samples.
- Perform process parameter experiments to optimize joint tensile strength.

Strategic Context:

- Falls under TARDEC Thrust area: Ground System Survivability
- Sub-area: Army Vehicle Light Weighting Campaign
- TSFW will be used by new Programs of Record (PORs) that require welding of steel to aluminum.
- The technology directly supports the TARDEC Strategy as a leap-ahead capability. It will also help ensure that newer lightweight requirements can be met without loss of performance.
- The project work product can easily transition to military stakeholders for utilization on new programs where dissimilar material joining is required. The technology also helps TARDEC's continual growth as the Joining Center of Excellence for the Department of Defense (DOD).
- Follow-on activity includes TARDEC pursuit of MANTECH support to further develop TFSW and Scribe Friction Stir Welding (SFSW).

Technical Barriers:

- Excessive FSW tool wear due to extremely hard steel (500 Brinell)
- Maintaining design tolerances of the joint surface while machining the high hardness steel bars. The barrier intensifies with the length of the steel bar.
- Thermal management of the process-induced friction heat within the bimetallic work pieces and weld fixture.
- The custom made FSW machine sometimes produces tool path errors or suffers breakdowns while performing bimetallic FSW.

Accomplishments:

- Two 18" and one 36" bimetallic friction stir welded plates were post-processed and made ready for TARDEC.
- Nine welded plates cut out from another three 18" bimetallic friction stir welded plates were sent to Metcut Inc for processing into 36 mechanical test samples. Metcut completed the task and returned the samples to Focus: HOPE.
- Completed heat treatment of the mechanical test samples per specifications provided by TARDEC.
- Completed testing of 2 sets of bend tests (10 samples each), 1 set of tensile test (10 samples) and 1 set of shear test (6 samples), and the results were submitted to TARDEC for review.
- Completed review of the broken FSW machine in consultation with the service engineers from Bond Technologies. It resulted in two different options for fixing the machine. Information on these options were then submitted to TARDEC for review and approval of a process for fixing the machine.
- While the machine was down, minor adjustments were completed on the welding fixture to accommodate entry and exit hole areas in the bimetallic friction stir welds. This would allow to retain the effective weld length to around 18" or 36".
- Brico Welding completed their original subcontract task. The results were reviewed and follow-on task for manual re-welding of plates were given to Brico. They completed the additional task as well, and delivered the welded plates to TARDEC. X-ray analysis of the welds showed no porosity.

Introduction:

Weight reduction and light-weighting of ground vehicle structures has become more important as manufacturers strive to improve vehicle dynamic performance and fuel economy. From this has arisen the need for new techniques and methods to apply lightweight materials during the design of vehicle components and structures. This need serves as the motivation for this work.

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Approach:

Based on a proof-of-concept project that successfully demonstrated the feasibility of joining high hardness steel to aluminum alloy using the FSW process (TARDEC R&D Contract #W56HZV-05-C-0721), this project expands upon those results to develop the tools, equipment, and manufacturing processes required to produce extended length (upto 36-inches) production-representative bimetallic weld joints. This project has three stages- a) FSW fixture development and installation b) FSW trials using four different tool configurations and conducting design of experiments (DOE's) to optimize process parameters for the best tool identified and c) Making 18 and 36 inch FSW samples, mechanical testing, advanced material characterization and reports development.

Results and Discussion:

In the first stage, the fabrication of a custom-designed FSW fixture was completed. This fixture was designed to hold multiple FSW samples at one time and also allowed use of thermal management techniques (as required) that were first demonstrated in the previous contract.

In the second phase, four different FSW tool design configurations (Tool A: 12.5 degree side tilt angle with single pass welds, Tool B: 12.5 degree side tilt angle with double pass welds, Tool C: 25 degree side tile angle single pass welds and Tool D: 36 degree side tilt angle single pass welds) were prepared, and tools were made using W-Re material for FSW experiments. FSW's were first made using trial process parameters for all four tools. The trial process parameters were based on prior experience of staff with the FSW machine and tool combinations. After inspecting the trial welds, it was found that Tool A produced the best welds. In order to identify and verify the optimal FSW parameter set for Tool A, additional L-9 Taguchi based FSW DOE's were completed.

In the last phase, currently underway, 18" and 36" long FSW's were made using the Tool A optimal process parameters. Select welds from this set were then mechanically tested (tensile, bend and shear), and the data was analyzed. The mean and standard deviation values observed from these tests are given below:

Bend Test:

Set 1: Flexure load at break, 1.496 ± 0.815 kN

Set 2: Flexure load at break, 1.404 ± 0.706 kN

Tensile Test:

Yield stress, 123.09 ± 8.775 MPa

Breaking stress, 139.23 ± 9.506 MPa

Breaking strain, 4.47 ± 1.17

Shear Test:

Shear strength, 73.285 ± 17.45 MPa

During the mechanical testing, the bend and tensile samples fitted well in the test setup. However, due to their thin and complex geometry, the shear samples had to be machined further to achieve shearing action during testing.

The mechanical tests show that both bend and tensile properties of the bimetallic FSW's have better consistency and robustness. The shear properties identified from the tests show larger spread (standard deviation) from the mean, however, the finding is attributed to less number of samples tested compared to bend and tensile.

Conclusions:

We investigated the use of four different W-Re FSW tool geometries for bimetallic friction stir welding of 0.5" thick 6061 aluminum alloy with 0.5" thick high hardness armor steel, and found that good welds of up to 36" length are doable. The observed challenges in the process are a) rapid tool wear, b) maintaining of tolerances during machining of high hardness armor steel coupons- especially as the length of the coupon increases from 18" to 36" and c) welding machine's ability to withstand loads resulting from the process. After completing all the experiments and analyzing the results, we have concluded that one of the four tools (Tool A), produces better welds than the others.

Plans for a) completing advanced characterization of the weld material and b) drafting final report material are being adjusted at Focus: HOPE in consultation with TARDEC. An approval of a no-cost, contract mod is required to proceed.

References:

1. TARDEC R&D Contract #W56HZV-05-C-0721 reports
2. TARDEC R&D Contract #W56HZV-14-C-0099 Quarterly AVPTA reports

Figures and Tables:

None

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AVPTA Technology Focus Area 2: Lightweight Structures & Materials

Multi-Material Joining (MMJ) – Advanced High Strength Steel (AHSS) Weld Wire

DOE-VTO TFA Lead: Sarah Ollila
TARDEC TFA Lead: Martin McDonnell

Principal Investigator:
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Demetrios Tzelepis

TARDEC
Product Lifecycle Engineering

Project Start: Q2FY14
Estimated Completion: Q4FY16

Objectives:

- Develop an innovative welding filler wire that can substantially reduce tensile weld residual stress and mitigate the susceptibility of hydrogen induced cracking (HIC).
- Develop residual stress measurement techniques using neutron diffraction for welded armor plates.
- Demonstrate the effectiveness of new filler wire to reduce HIC on selective welding conditions.
- Determine Base Mechanical Properties of New Weld Wire.

Strategic Context:

- The project was initiated to resolve hydrogen embrittlement during welding of armored vehicles by creating a weld wire that would produce a hydrogen embrittlement-resistance microstructure, with an added bonus that the welding process will produce compressive residual stress, instead of tensile residual stresses at the weld toe. This would improve fatigue performance which is an interest in the automotive industry.

- The weld wire can be used across all armor steel protected military vehicles, therefore the wire will be applicable to the sustainment of legacy vehicle as well as new program of records.
- The innovative weld wire would also include potential benefits in other industries and defense applications such as hydrogen embrittlement mitigation and weld residual stress and distortion in shipyard.

Accomplishments:

- Established three experiment weld wire chemistries, and successfully produced two 0.041 in. LTPT weld wires, HV1764 and HV1766. Both weld wires were resistant hydrogen embrittlement and can be welded in ambient conditions. A patent application was filed for these families of wires in 2015.
- LTPT weld wire HV1766 produced compressive residual stress at the toe of the weld, and showed an overall decrease in the residual stress distribution in the weld and heat affected zone. Results were presented at two conferences, NMC Shiptech, AWS FABTECH.
- With respect to tensile properties, LTPT weld wire HV1766 is over matched to MIL-DTL-12560, i.e. failure will occur in the base metal and not within the weld zone, or heat affected zone. Current commercial wires are opposite; failure occurs in the weld zone.
- Charpy testing showed a relatively low impact toughness of the weld when compared to the RHA base metal. The reduction in impact toughness is thought to be produced by inclusions during the welding process. Preliminary testing of Charpy impact, of all weld metal samples, showed the same. Currently investigating a change in welding gas from a 95-5 Argon/CO₂ to a 100% Argon to improve the toughness. Other means of toughness improvement by optimizing the weld wire chemistry are being also planned.

Introduction:

It is well established that three essential conditions must co-exist for HIC – (i) presence/absorption of hydrogen from welding operation or environment, (ii) sensitive hardened microstructure, and (iii) high tensile residual stresses. Weld residual stresses develop in a welded structure as a result of the non-uniform thermal expansion and contraction of the base metal during welding operation. The weld region typically cools last in the entire weldment. As it cools from the melting point of the materials, the weld region shrinks. It is such on-cooling shrinkage that results in the formation of high-tensile residual stresses in the weld region that can reach or even exceed the yield strength of the base material.

Approach:

The innovative weld wire development was based on the principle that a volumetric expansion process taking place during the cooling period could negate the effects of thermal shrinkage. One such volumetric expansion results from the phase transformation of austenite to a low temperature phase such as ferrite, bainite, martensite, or more likely a mixture of these low temperature phases in a steel. The effectiveness of the volumetric expansion to negate the formation of high-tensile residual stress depends on the extent of the volume expansion and

temperature range in which the allotropic phase transformation takes place. The formation of martensite, especially at a temperature range close to but above the ambient temperature (or the intended service temperature of the weldments), is most effective.

This project is to develop a special welding filler wire which utilizes low temperature phase transformation (LTPT) to reduce the high-tensile residual stresses in the weldments of high-strength steels to prevent HIC. The filler wire makes it possible for “in-welding-process” HIC control, thereby eliminating the need for pre or post weld heat treatments. This reduces the fabrication cost and enables the use of high-strength steels based on the application needs without the concerns of HIC. Weld filler wire chemistries are systematically designed based on the LTPT principle and experimentally evaluated in the project to determine suitable weld filler wires to prevent HIC specific for armor applications.

Results and Discussion:

In 2016, the project concentrated on collecting additional data for mechanical properties of the experimental weld wires, further residual stress studies, and disseminated data to industry through two conferences, NMC Shiptech, and AWS FABTECH. Finally, patent pending status was awarded for this family of weld wires. This protection of the intellectual property will allow for further dissemination of weld wire performance through multiple peer reviewed publications.

Residual stresses were also measured at ORNL’s High Flux Isotope Reactor (HFIR) using neutron diffraction for Heat HV1766 welded to MIL-DTL-12560 in a Y-Groove configuration. Figure 1 shows the results of the neutron diffraction experiments. The HV1766 weld wire showed a decrease in the residual stress distribution around the weld zone. At the toe of the weld the stresses were compressive or near zero. This compressive stress would produce a more fatigue resistant wire and contributes to the increase in the resistance to hydrogen embrittlement over the conventional ER 100 wire. Currently surface stresses are being measured on unrestrained plates using multiple passes for both HV1766 and HV1764 for both the MIL-DTI-46100 and MIL-DTL-12560 material. The results are due by November 2016.

TARDEC produced 21 in. x 14 in. mechanical test plates using the HV1766 wire and 0.5 in. MIL-DTL-12650. Lower heat input welding parameters were chosen. Figure 2 tensile properties shows of weld metal. The properties were measured in the longitudinal direction of the weld. The tensile strengths ranged from 140-160 KSI with a total elongation of 7-8%. This is similar to the MIL-DTL 12560 material.

Impact properties were also measured with relatively low the Charpy values (Figure 3). It was decided late in the 2016 to switch welding gases from a 95-5 argon-CO2 mixture to a 100% argon mixture. The results are due by the end of November 2016. Other means of toughness improvement by optimizing the weld wire chemistry are being also planned.

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Conclusions:

Our current approach has shown the feasibility of a new HIC resistant-high strength welding filler wires. The weld wire HV1766 produce weldments with favorable residual stress distributions with respect to hydrogen embrittlement and fatigue performance. The following work will be continued in FY17. Further develop welding process to increase the toughness of the HV1766 weld wire. Complete the characterization of the HV1766 weld wire and the HV1764 weld wires, and submit final report.

Figures and Tables:

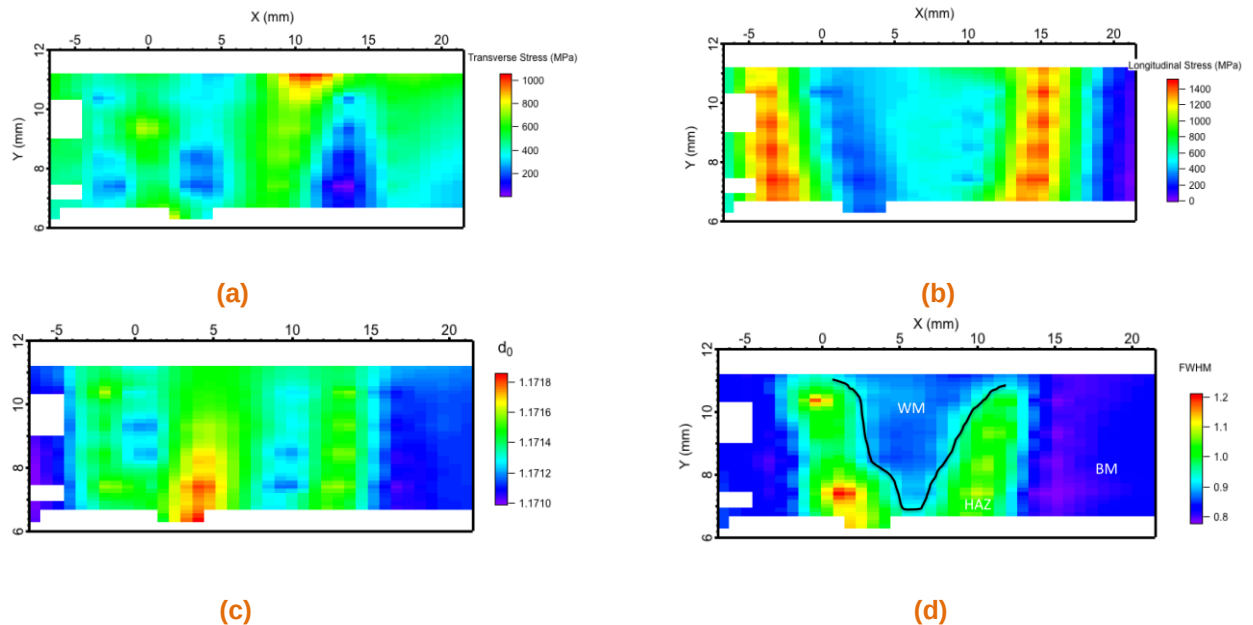


Figure 1. Residual stress distribution of Y-groove plate welded using LA-100 (a) transverse direction (b) longitudinal direction (c) distribution of stress free lattice spacing (d) distribution of FWHM

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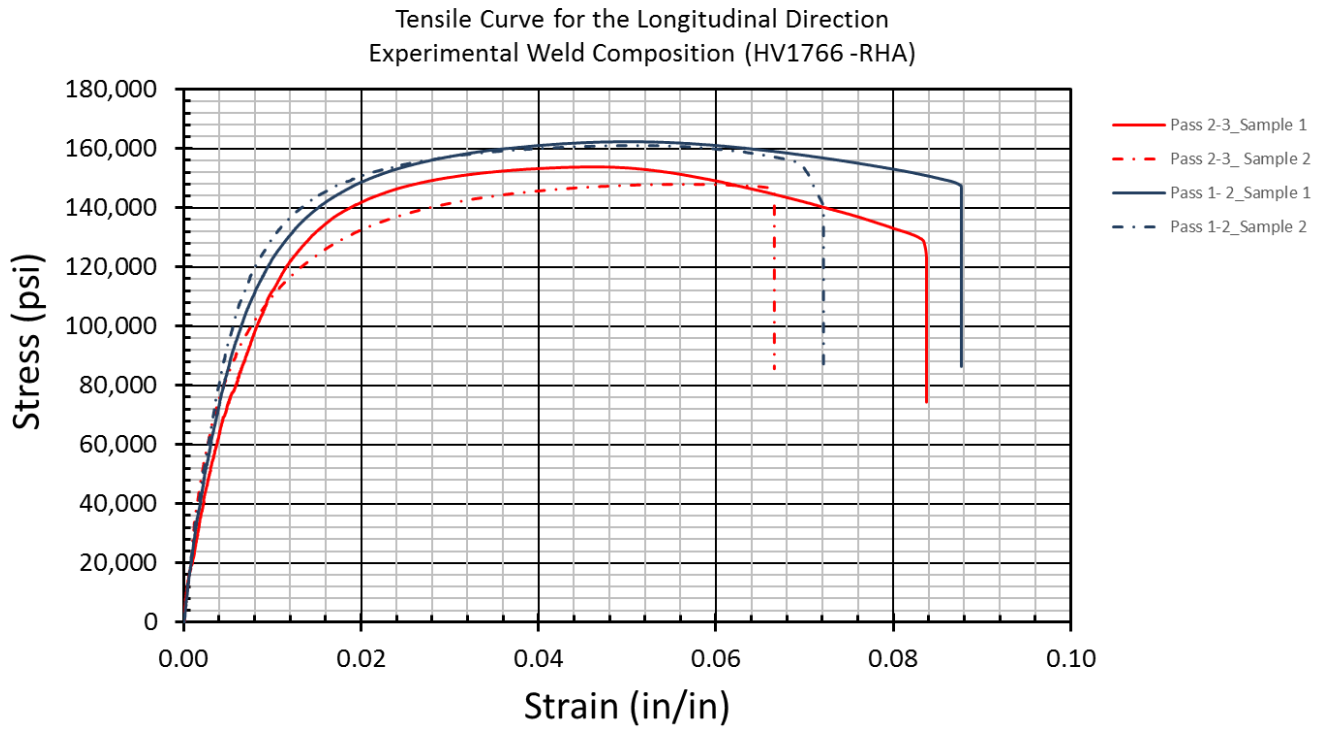


Figure 2. Tensile properties of multiple pass weldment HV1766and RHA.

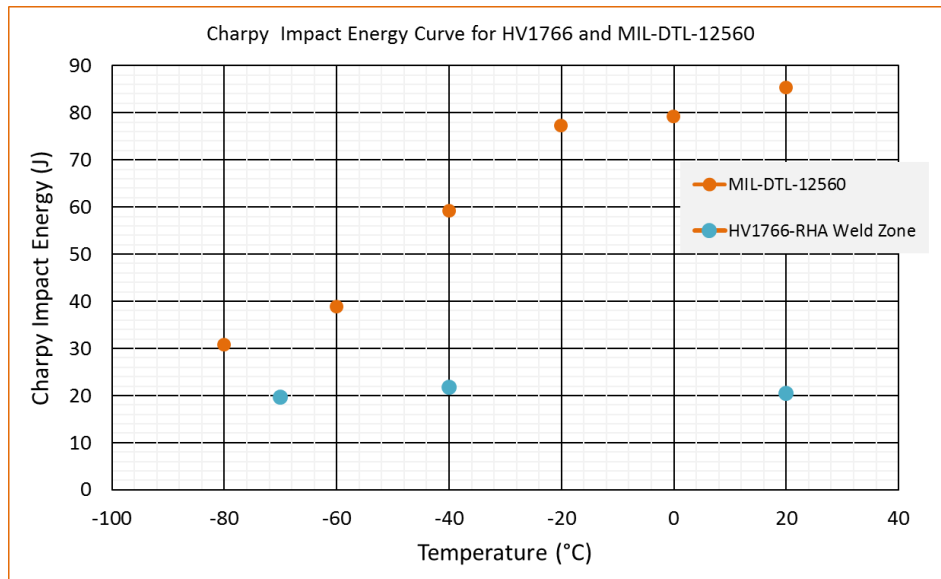


Figure 3. Charpy Impact Energy Curve for HV1766 and the MIL-DTL-12560 base metal.

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AVPTA Technology Focus Area 2: Lightweight Structures & Materials

**Multi-Material Joining (MMJ) – Weld Wire Characterization in Welding
Advanced High-Strength Steels (AHSS)**

DOE-VTO TFA Lead: Sarah Ollila
TARDEC TFA Lead: Martin McDonnell

Principal Investigator(s):
Mr. Matthew Rogers

Affiliation: TARDEC
Material Integration & Application Team

Project Start: Q1FY14
Estimated Completion: Q4FY17

Objectives:

- Understand the joint quality and welding process efficiency of welded armor steels.
- Establish weld wire selection criteria for the new MIL-Standard on the welding of armored steel.
- Provide practitioners a point of comparison between current joining practices and future welding practices.
- Create validation data for ballistic and blast models of welded armor plates.

Strategic Context:

- The project data will transition and be used by both TARDEC engineers and vehicle manufactures to further optimize vehicle designs. The data will identify optimal weld wire / material combinations to maximize weld filler material properties. The information will be transitioned to OEMS and suppliers through the military weld standard.
- The project supports TARDEC's Value Stream 2 by providing PM's with data and standards for improving weld quality for all steel vehicles. The same data and standards can be transitioned to the automotive industry.
- The project continues to build on the AVPTA MMJ investments in making TARDEC a joining center of excellence. The level of detail and fidelity of study speaks to TARDEC's in-depth expertise in welding.
- Future plans are to expand the study to include aluminum materials (2xxx, 5xxx, 6xxx, and 7xxx).

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Accomplishments:

- Phase 1 Testing 50% Complete
- Phase 2 Testing 75% Complete
- Phase 3 Testing 100% Complete
- H2 Testing and Final H2 Report Complete

Introduction:

The chemical and mechanical properties of armor steel used by the US Army are similar to advanced high strength steels used in the automotive industry. The ultimate tensile strength ranges from 150 ksi to 300 ksi depending on the armor grade selected. The last MIL standard for welding armor was canceled in 1998 and replaced with the Ground Combat Vehicle Welding Code (GCVWC)-Steel, which has never been updated and has no engineering guidance for the selection of weld wire. Additionally, neither the old MIL standard nor the GCVWC-Steel include any recommendations based on newer armor grades and new welding techniques. There are also no published industry guidelines for welding of advanced high strength steels, which the government could use to weld armor. This has led to a proliferation of welding techniques by the defense contractors, which in turn has led to a general decrease in weld quality and the proliferation of defects, such as cracks induced by hydrogen embrittlement.

Performance of welded joints is critical to the performance and reliability of ground vehicles. The performance depends on many factors associated with the welding. One key factor is the type of weld wire, of which there are many. A weld wire is classified by weld process and tensile strength. The preferred process for welding plate armor in ground vehicles is Gas Metal Arc Welding (GMAW) pulse. Weld wire tensile strength ranges from 70 ksi to 140 ksi; some ground vehicle manufactures have even used austenitic stainless steel filler metals. Unfortunately, the weldments made from these wires in combination with modern armor materials have not been characterized. There is also a general lack of knowledge of the mechanical and ballistic performance, in terms of joint efficiency, of these wires. Joint efficiency is defined as the ratio of the properties of the welded armor to the properties of the base metal armor. If the joint efficiency of each weld wire is known, then proper filler metal selection criteria can be established and implemented through a the new weld standard.

In addition to establishing selection criteria for the welding of armor steel, the data obtained in this study will be used to validate material models for ballistic and blast modeling and simulation. This data can be used by both TARDEC engineers and vehicle manufactures to further optimize vehicle designs.

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Approach:

The project is divided into three phases:

Phase 1: Investigate the mechanical and metallurgical properties of welded armor using various weld wires:

This phase involves robotically welding MIL-DTL-12560 class1, MIL-DTL-46100 class1, and ASTM A514 Grade A to themselves in 14" x 21" x 1/2" single V-groove sample. Filler materials are solid wire, stainless steel, and metal core filler. Various tensile strengths ranging from approximately 70ksi-140ksi will be used. All samples will be welded internally at Center for System Integration (CSI). The samples will then undergo tensile, hardness, fatigue, charpy impact, hydrogen embrittlement (see Figure 1). Once this is complete the samples will be ranked for performance. The highest performers will move to Phase 2.

Phase 2: Perform high strain rate events using a ballistic shock test with a welded H-Plate.

This phase will involve taking the highest filler performers from *Phase 1* and robotically welding them into a 3'x 3' x 1/2" H-plate configuration. The same single V-Groove configuration will be used throughout this test as well. Once the plates are welded and radiographically tested they will be sent over to the TARDEC SABL lab for Ballistic Shock testing (see Figure 2). If the samples pass they will be used for *Phase 3*.

Phase 3: Perform penetration testing to determine magnitude of vulnerability.

This phase will involve taking the performers from *Phase 2* and robotically welding 2' x 2' x 1/2" single V-groove plates. Penetration testing will be conducted to determine the joint efficiency as defined by the magnitude vulnerability (see Figure 3). These tests will be performed with a high speed camera and flash x-ray to record the dynamic deformation during the ballistic shock test. Understanding the dynamic deformation response is crucial to improving our understanding of weld responses to high strain rate events.

Results and Discussion:

In the first year the overall study plan was completed and the welding material and weld wires procured. In addition, it was necessary to develop an automated manner to weld standard I plates and H plates for testing. Figure 1 shows the hardware fixture that was developed to robotically weld the large sample of I and H plates. Figure 2 shows a completed I plate weld, and Figure 6 shows how an H-Plate looks by comparison.

One issue that was not anticipated was that the MIL-DTL-46100 (high hard) material became highly magnetic from the shoot penning cleaning process. This required adding the additional step of demagnetizing the material before welding to prevent arc blow (see Figure 4).

The *Phase 1* I plates welding has been completed. Figure 5 shows a sample hardness scan of a completed weld zone. Figure 6 shows how all the weld characterization samples are cut from a single plate. Three samples will be cut from different plates for each weld wire / parent

material combination to obtain statistical validity of the results. *Phase 1* is currently about 50% complete. For the tensile samples one of the four sets of tensile bars for every combination has been complete. We currently have data to understand what the trends look like. As tensile strength goes below 80ksi or above 120ksi ultimate tensile strength yield strength properties begin to change. It is too early to tell but I believe that there will be a level that will be acceptable ranging from 80ksi to 100ksi.

Phase 2 is at 75% complete. Range time to complete this task is difficult. The range has about 25 H-Plates left to shoot. I add Digital Imaging Correlation (DIC) software to the testing in order to understand the deflection on the steel at high strain rate. Completion for this will be no later than May 2017.

Phase 3 is 100% complete and the final report is being completed. Final report due early 2017.

Hydrogen Embrittlement study is complete final report was just finished on Nov 4th 2016.

Conclusions:

The *Phase 1* plates will be tested and analyzed. The remaining *Phase 2* plates will take approximately 9 months to weld. Once the data is collected, it will be statistically analyzed and provide input to the development of a new MIL-STD-3040 for welding. MIL-STD-3040 will utilize the data and testing criteria to develop mechanical acceptance criteria.

This data will transition and be used by both TARDEC engineers and vehicle manufactures to further optimize vehicle designs. This data will transition to Industry, PM's, Depot's, and Arsenal's through the new welding mil standard, by creating filler metal selection charts. The data from this project will also be easily transitioned to help industry, such as the automotive and heavy equipment companies, in the selection of weld filler materials for their types of AHSS due to the similarities in properties. The data obtained in this study will also be used to refine material models for modeling and simulation

References:

None

Figures and Tables:

Test	Locations	Time Frame
Robotically welded samples	TARDEC CSI weld area	FY14
Tensile Testing	TARDEC Metallurgical Lab	FY14/FY15
Hardness Testing	TARDEC Metallurgical Lab	FY14/FY15
Charpy Impact	TARDEC Metallurgical Lab	FY14/FY15
Fatigue Testing	Mississippi State University	FY14
Hydrogen Embrittlement Test	Oak Ridge National Lab	FY15

Table 1. Phase 1 Test, Test Location and Timeframe

Test	Locations	Time Frame
Robotically welded samples	TARDEC CSI weld area	FY14/FY15
Radiographic Test	ANAD	FY15
Ballistic Shock Test	TARDEC GSS SABL	FY15/FY16

Table 2. Phase II Test, Test Location and Timeframe

Test	Locations	Time Frame
Robotically welded samples	TARDEC CSI weld area	FY15
Radiographic Test	Outside Contractor	FY16
Penetration Test	TARDEC GSS SABL	FY16

Table 3. Phase III Test, Test Location and Timeframe



Figure 1. Fixture for Robotic Welding of Phase I Plate



Figure 2: Phase II H-Plate Clamped and Ready for Welding



Figure 3: Penetration Testing Phase III

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Figure 4. Demagnetizing Process

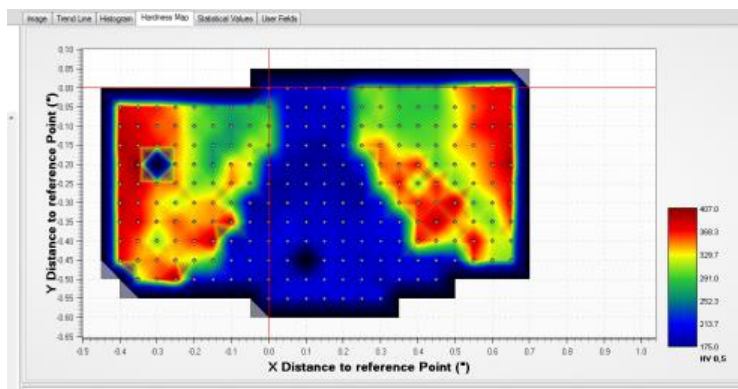


Figure 5. Sample of Micro hardness profile



Figure 6. Phase I-Plate Marked Samples for Standardized Weld Characterization Tests

AVPTA Technology Focus Area 2: Lightweight Structures & Materials

Multi-Material Joining (MMJ) – High Strength Weld Wire Development Suitable for High Strength 6XXX Aluminum Alloys

DOE-VTO TFA Lead: Ms. Sarah Ollila
TARDEC TFA Lead: Mr. Martin McDonnell

Principal Investigator:
Mr. Matthew Watson

Affiliation:
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Alcoa Technical Center
100 Technical Drive
Alcoa Center, PA 15069-0001

Project Start: Q3FY14
Estimated Completion: Q3FY17

Objectives:

- Develop a weld wire for welding high strength aluminum plate, particularly 6055; such that the weld joints exhibit improved mechanical properties and corrosion resistance over the incumbent weld wire material.
- Refine the chemistry of the weld wire in an effort to optimize the corrosion and mechanical properties of the resulting weld joint.
- Fusion weld aluminum alloy materials (5083 and 6055) with the newly developed high strength filler wire.

Strategic Context:

- Permits the light weighting and improved performance of new vehicles, as well as increased protection for the Warfighter, due to a 20% strength increase in 6xxx alloys
- Improves the maintainability and repairability of legacy vehicles.
- Provides a cost effective solution and enables design flexibility in material choices for high performance combat and heavy transport vehicles.
- Attractive for commercial transportation applications to cost effectively save weight.

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Accomplishments:

The production of small volumes (50-100 lbs.) of filler wire for initial gas metal arc (GMA) welding evaluations, including weldability and mechanical property evaluations, has proven to be a time consuming activity that involves 5 steps and multiple vendors:

- Cast ~100 lb. billets (Alcoa) of C138H and C139H
- Billets were homogenized (Alcoa), cropped and scalped, and cut to length
- An annealing practice will be developed for C138H and C139H
- An extrusion practice was developed based on the composition of the material and capabilities of the extrusion press
- The technical information package and quoting materials was completed to place Alcoa Forging and Extrusion (AFE) Pimalco (Chandler, AZ) under contract to extrude our C138H and C139H filler alloy billets.
- All billets were milled, sawn and marked according to Pimalco's requirements, and shipped.
- Tests were performed to ensure environment, health and safety (EH&S) compliance
- Extrusion dies were designed and ordered
- Extrude billets to 0.75" rods (Pimalco)
- The 0.5" rods will be drawn down to 0.118" wire and coiled (Beneke)
- The 0.118" wire will be drawn down to the final 0.062" diameter by Hobart
- Written report on the progress to date with the 5k/6k weld wire development focusing on the technical difficulties encountered.
- Potentially adding 7085 weld wire development to the SOW and extending the period of performance

Introduction:

High strength 6XXX aluminum alloys, such as 6055, have approximately 20% higher strength than currently used aluminum alloys. They offer the potential to significantly improve performance and reduce weight and cost. However, when welding 6XXX high strength alloys, the only commercially available filler wires that can be used to weld these alloys without cracking produce welds with limited shear strength and ductility¹, which in turn limit their capability to withstand blast type of loads. Because the joints produced with these filler wires are so much weaker than the parent material, the full benefits of the high strength 6xxx alloys cannot be realized. As such, the thickness of the components must be designed to compensate for the weakness of the joining method used, resulting in parasitic materials and increased weight. The increase in weight results in an increase in fuel consumption, an increase in drive train and suspension requirements, and a loss in performance. In addition, when welding these high strength alloys to 5XXX (e.g. 5083) parts, the use of 4XXX type filler leads to formation of brittle MgSi₂ at the fusion zones of the welds with the 5XXX parent metals. On the other hand, when welding such high strength 6XXX/5XXX alloy combinations with Mg based 5XXX filler alloys (e.g. 5556, 5356, 5183), the formation of Mg/Cu low melting eutectics at the fusion zones of the welds leads to their cracking. Improved joining methods are therefore needed so that these high strength materials can be joined in a fashion that optimizes the vehicle manufacturing system.

To address this need, Alcoa is developing a number of weld wires that would result in higher strength weld joints over the incumbent weld wires.

Approach:

In the past, the extrusion step was performed at an Alcoa facility on an extrusion press that was recently shut down. As such, Alcoa has been working to identify an alternative supplier for extruding the 4 prototype billets that were cast in 2015. Extrusion trials have been performed at an outside vendor and at another Alcoa location but with less than desired turnaround times and/or quality.

During Q1FY16, two (2) alternative solutions were identified and explored. First, the team identified an Alcoa location in Pennsylvania that can extrude the billets to 0.75" rods. Alcoa then confirmed with Vendor 2 that they can still draw the 0.75" rods to 0.118" wire. If this route is chosen, extrusion dies will need to be ordered since they do not currently exist at the location, and a plan has been established for this option. Alternatively, Alcoa has reached out to the facility that was initially extruding the material to see if the press can be operated again. In this case, this location may also be able to draw down the rods to 0.118" wire, which would also help improve the overall turnaround time of producing the material. A decision is expected to be reached within the next week, at which point the processing of the wire will continue.

During Q2FY16, an alternative solution was identified and plans were formulated to extrude the billets to 0.75" rods. Since this is slightly larger than the previous 1/2" rods, Alcoa worked with Vendor 2 to confirm that they can draw the 0.75" rods to 0.118" wire and solicited quotes for this step in the process.

During Q3FY16 the technical information package and quoting materials were completed to place Alcoa Forging and Extrusion (AFE) Pimalco (Chandler, AZ) under contract to extrude the C138H and C139H filler alloy billets. All billets were milled, sawn and marked according to Pimalco's requirements, and shipped. AFE Pimalco agreed to a schedule that would enable them to extrude these billets in late June.

During Q4FY16 Alcoa Forging and Extrusion Pimalco (Chandler, AZ) successfully extruded the C138H and C139H filler alloy billets down to 0.5" diameter rod, with minor material losses.

Results and Discussion:

The C138H and C139H compositions are significantly higher in certain alloying elements than traditional aluminum 5XXX filler wire² alloys. Therefore, the flow stress (yield strength) of the material is higher than that of traditional filler alloys. These compositions also work harden more than traditional 5XXX alloys, leading to high tensile stresses during the drawing process. It is due to the higher strength and work hardening of these compositions that the processing from billets to useable weld wire has been so fraught with difficulties. A more conservative approach (less reduction in each drawing pass) has been proposed.

Conclusions:

Further delays are expected with the 5XXX filler alloy development. An interim report on the technical difficulties encountered will detail the problems with these weld wire compositions. Alcoa and TARDEC are considering adding 7085 weld wire development to this effort.

References:

- 1 – <http://www.dtic.mil/dtic/tr/fulltext/u2/a622461.pdf>
- 2 – <http://www.azom.com/article.aspx?ArticleID=2804> (example)

Figures and Tables:

None

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AVPTA Technology Focus Area 2: Lightweight Structures & Materials

Multi-Material Joining (MMJ) – Laser-Assisted Cold Spray

DOE-VTO TFA Lead: Ms. Sarah Ollila
TARDEC TFA Lead: Mr. Martin McDonnell

Principal Investigator:
Dr. Pravansu Mohanty

Affiliation:
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1058 WOLVERINE TOWER
3003 S. STATE ST
ANN ARBOR MI 48109-1274

Project Start: Q4FY14
Project Completed: Q1FY17

Objectives:

- Vehicle weight reduction via coated Aluminum brake rotor.
- Exploration of alternative alloys to reduce brake fading.

Strategic Context:

- Coated aluminum brake rotors will support sustainment of existing Programs of Record (PORs) and be available as an option for next generation vehicles.
- The technology directly supports the TARDEC Strategy for the sustainment and light-weighting of legacy and next generation POR vehicles.
- TARDEC Ground Systems Survivability (GSS) will be able to utilize the new light-weight armor applicable to legacy and next generation POR vehicles.
- Follow-on activity is conditional to results of pending testing and evaluation.

Accomplishments:

- Dynamometer testing of coated aluminum brake rotors
- Large area deposition modeling to reduction production time

Introduction:

The ability to strategically position a desired material can lead to lighter, robust components. For ex: A hard dense material in conjunction with a lighter material can enhance performance and weight reduction. A ductile material surrounding a hard material can improve impact resistance. While the applications might appear diverse, the common barrier to these

multi-material systems boils down to the ability to hold them together. This joining technique and choice of materials then determine structural integrity and useful life of the component.

Conventional joining techniques rely on melting to fuse components together. Difference in melting points and formation of brittle intermetallic phases limit its use with dissimilar materials. The choice of materials also plays an important role. Galvanic incompatibility can accelerate galvanic corrosion. Mismatch in coefficient of thermal expansion can also cause excessive stresses leading to premature component failure.

The focus of this project is to enable effective use of multi-material components to achieve weight reduction in military vehicles. This can increase mission lengths or payload. Optimization of two components; brake rotor discs and renewed search for alternative alloys are addressed in this investigation.

Brake Rotor Discs - Coated Aluminum Brake Rotor:

Brake rotors constitute a heavy unsprung mass that acts as a heat sink to dissipate the kinetic energy of the vehicle in order to decelerate or stop. In addition the rotor surface provides stable friction across its operating regime. Weight reduction in rotors can increase mission lengths (via fuel efficiency) but also ride and maneuverability. Coated Aluminum brake rotors present a viable light weighting solution. The coating withstands the grunt braking action while the aluminum serves an efficient heat sink and keeps temperatures low. Key issue with this concept is the lack of feasible joining process and compatible material system. The present investigation has developed a potential coating material and deposition process to fabricate coated aluminum brake rotors.

Approach:

Process:

The University of Michigan has developed a novel Co-axial laser assisted supersonic sintering process (CLASS). This solid –state deposition technology overcomes the hurdles of multi-material joining process: - melting point, formation of intermetallics and thermal degradation. Akin to cold spray technology, powders of desired materials are accelerated to target area at supersonic velocities. At these conditions, the powder undergoes adiabatic shear straining to create micro jets at the interface to create metallurgical bonds. A coaxial laser beam irradiates this foot print to relieve excessive stresses to prepare for next layer of deposition. The novelty of the process lies in the ability to switch the laser beam as primary deposition source. Here at significantly lower particle velocity; the process can create finer deposited features. The CLASS process has been utilized for this investigation. (Figures 1 A&B).

Aluminum Alloy Selection:

Unlike conventional grey cast iron rotors, the useful life of coated aluminum rotors is clearly limited by the coating thickness threshold. This is necessary to prevent localized hot spots and subsequent warping. If designed conservatively, the potential weight savings can be upwards of 50%. The Silverado rotors were reversed engineered (Figure 3) to match GDOT

requirement. Al356 rotors were cast and manufactured according to the GDOT rotor specification. The obtained aluminum casting is shown in Figure 4. Previously, rotors were cast using an Al398 high temperature alloy. While Al398 alloy has better high temperature characteristics (Figure 2), porosity in the casting could not be avoided without veering into casting process optimization. Hence, Al356 alloy was used to manufacture rotor castings for preliminary coating deposition and testing.

Coating Material Selection:

The Fe-Mn-Al material system has been thoroughly investigated and is considered as a potential coating material for brake rotor application [1]. The work hardening property of the Mn based ferrous alloy system results in plastic deformation under impact loading with abrasion or erosion. This mechanism obviates the possibility of brittle fracture and spalling [2]. Manganese is an austenite former and a cost effective replacement for Nickel. Disadvantages of manganese are the tendency to segregate forming beta manganese and its high affinity for oxygen at higher temperature [3]. This often results in the alloy with depleted Mn content. This alters the stacking fault energy (SFE) leading to formation of martensitic phases which could be unwarranted and detrimental. Aluminum also helps increase the SFE. Therefore it stabilizes the austenitic phase and prevents formation of martensitic phases. At Higher levels of aluminum, the formation of a continuous passive layer has been shown [4,5]. Chromium additions to Fe-Mn Alloys have been widely studied as means to improve the corrosion properties of this alloy [6,7]. Chromium also increases the yield strength or the flow stress thus enhancing wear property [6]. Carbon and Nitrogen are two other important elements widely researched in Ni-free austenitic alloys. Both these elements have higher solubility in austenite matrix. The disadvantage of these interstitials is precipitation. The maximum amount of carbon that can be added was limited to 1.2% [7] Nitrogen up to .22wt% has shown to reduce work-hardenability [8]. Carbon has been shown to precipitate at 450°C [9]. Carbon was however added as it affects the critical resolved shear stress which is necessary for twinning [7, 9].

Thus, Fe-Mn-Al-Cr-C Alloy system forms a suitable framework for wear resistant alloy for a brake rotor application. The role of manganese will be to ensure the stability of austenitic phase at all temperatures and compensate for its affinity to oxidize. By Varying Aluminum and Chromium the galvanic potential of the alloy will be brought to match that of aluminum. The role of carbon will be to enhance twinning tendency. Its precipitation will result in strengthening of the alloy and lubrication preventing galling.

Optimization of Fe-Mn Alloy Composition:

The Fe-Mn alloy (B95 rockwell hardness) was modified from previous compositions to improve the overall deposition efficiency of the powder while also meeting target brake performance. Different variations of the Fe-Mn alloy can be seen in Table 1.

Development of Alternative Alloy for Fe-Mn Steel:

Austenitic steel alloys have several advantages from a metallurgical standpoint. Their FCC structure is very tough and ductile down to absolute zero. These steels also do not lose their strength during high temperatures which can occur during severe braking conditions [10].

Two alloys from the Nitronic series N50 and N60 were chosen based on the higher hardness when compared to high Mn alloy. Metal to metal galling resistance for N50 and N60 are typically higher than the 316SS. Due to this reason they can be used for brake rotor applications. These alloys also have a higher hardness and are more corrosion resistant than the typical 316 and 317 stainless steel. Their yield strength is also much higher than 316SS. Unlike many of the typical austenitic steel these do not become magnetic when cold worked. Much of all this is attributed to the composition of both these alloys [11]. The typical compositions of the Nitronic 50 and 60 can be seen in Table 2.

Results and Discussion:

Dynamometer Test Results:

The coated aluminum rotor was tested in 2015 Chevrolet Tahoe Police Front platform. A SAE J2784 FMVSS 135 testing protocol was followed. The tests include burnish, effectiveness, baseline, fade and recovery. The results of test are plotted in Figures 5 and 6. The testing comprised of 16 sequences and are shown individually in these figures. The critical factors namely the surface temperature, brake pressure, effectiveness and average friction during these test cycles are plotted in the figure.

The photographs of the rotors post testing is presented in Figure 7. There was substantial difference between the inboard and outboard surfaces of the rotor. The inboard surface presented a cleaner burnished surface with a consistent transfer layer from the brake pad. The cross-sectional images from both surfaces is shown in Figure 8. Consistent with photographs the inboard coating surface shows considerably less damage. In order to understand the cause for failure in the coatings in terms of cracks and delamination, results are compared with previous successful rotor tests. Figure 9 shows the results of coated aluminum rotor tested in a passenger car platform.

There are two modes of failure. These arise from excessive temperature and friction. To investigate further, the surface temperature plots from three front brake rotor tests are plotted in Figure 10. These include the coated aluminum rotor (Figure 7), its cast iron benchmark and the successfully tested coated rotor (from the passenger tests, Figure 9). The minimum and maximum frictional coefficients from the coated aluminum rotor and its cast iron version are presented in Figure 11.

All rotors experience three high temperature cycles. These occur during high speed effectiveness measurement and during heating snubs. Corresponding to sections – 7.6, 7.13 and 7.14 in Figures 5 and 6. The temperatures achieved by both coated aluminum rotors are similar. This suggests that the cause of failure is not directly related to temperature. From Figure 11. It is seen that until about 50 braking operations (stops) the frictional performance of both rotors are identical. During this period the rotor undergoes one of three high temperature cycles. After this period the frictional coefficient begins fluctuating. This indicates that the failure began at this period.

In comparison with the passenger car tests, the number of burnish cycles in the current tests was low. The burnish cycles is necessary in order to generate a stable friction layer. During this stage a transfer layer comprising of materials from both mating surfaces is formed. Instability in

this layer can result in excessive wear debris. In present tests, one possible reason for failure could be the breakdown of this layer which could have resulted in frictional instability, recorded after about 50 stops. The wear debris then resulted in instable friction layer as shown in Figure 11. The debris could have resulted in abrasive action which is consistent with the surface of the outboard rotor surface.

Deposition Rate:

As indicated previously, coating deposition efficiency is being continuously improved. One of the barriers to significant reduction in deposition duration is the ratio of per layer thickness to overlap.

A larger nozzle was fabricated to attain higher powder throughput. While dense coatings were obtained the decrease in production time was modest. This is because the coating deposition occurs in layers. Each layer produces a determined coating thickness. Hence in order to speed up, the number of layers must be reduced. This means that each layer requires even multiples of deposited thickness. Further, there exists a threshold as increasing thickness prevents even overlap. In addition to overlap, overspray is also necessary in order to achieve said thickness.

One way to boost the production rate in high volume applications such as these is to adapt the cold spray nozzle into wide area deposition platform. Development of such a nozzle is in progress. Figure 12 shows the CAD and results from numerical analysis predicted the geometry of such a nozzle to obtain substantial coverage.

In addition to improvement in nozzle geometry, the expansion ratio of the nozzle was tailored for Fe-Mn powders. This is the ratio between, exit to throat area of the nozzle. This ratio determines the operating pressure of the nozzle just before the gas leaves the exit. This pressure dictates the operating regime of the nozzle such as under expanded, perfectly expanded and over expanded modes. This ratio regulates the intensity of shockwave at the exit of the nozzle. It also controls the exit gas temperature which is beneficial in imparting annealing effect on the deposited coatings. The deposition weights obtained from nozzles with three expansion ratios is presented in Figure 13. It can be seen that a higher rate is obtained from Nozzle 3 with lower gas consumption.

Conclusions:

Coated aluminum rotors were tested on a brake dynamometer. A Chevrolet Tahoe-Police front rotor test bench was used to conduct the appropriate FMVSS 135 tests. The tested rotor did not perform as well as previously demonstrated results on a passenger car (sedan) test bench. The cause of failure was attributed to unstable friction transfer layer which resulted in excessive debris causing abrasion. The abrasion was evident physically on the rotor surface. A revised pad material or changes in the FMVSS script to incorporate higher number of burnish stops to improve transfer layer properties is recommended.

To reduce production time of the coated rotor, a multi nozzle arrangement is being developed to improve coverage and overcome issues leading to overspray and incorrect overlap. In the meantime, nozzle geometry is being optimized for the Fe-Mn coating material.

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- [12] Smt.Sandvik.com

Figures and Tables:

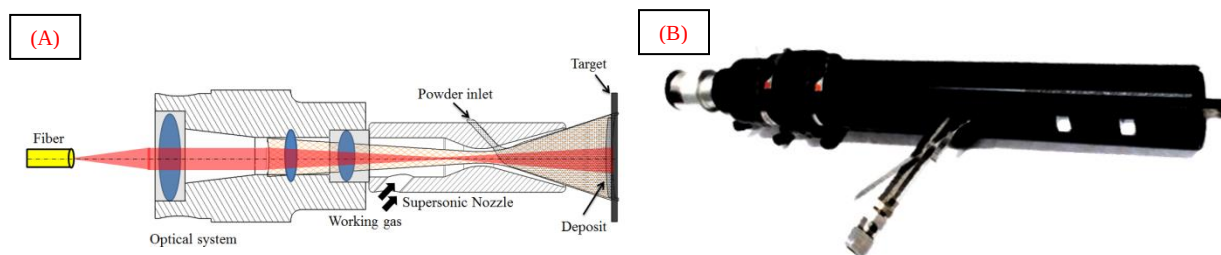


Figure 1. (A) Schematic of CLASS process (B) CLASS Prototype.

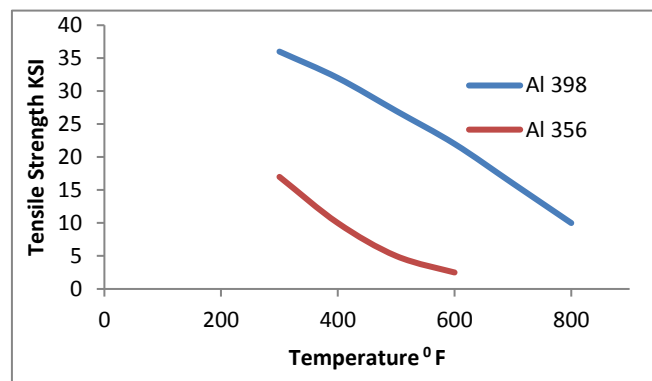


Figure 2. Elevated Temperature property Aluminum Alloy

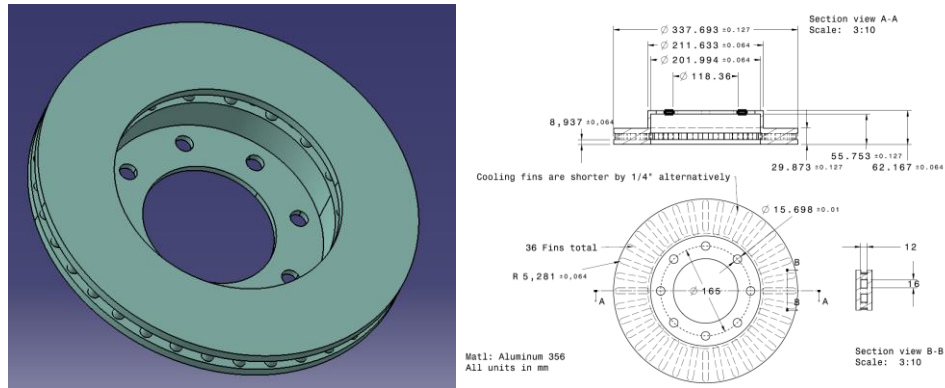


Figure 3. Al356 Brake Rotor Casting Specification.

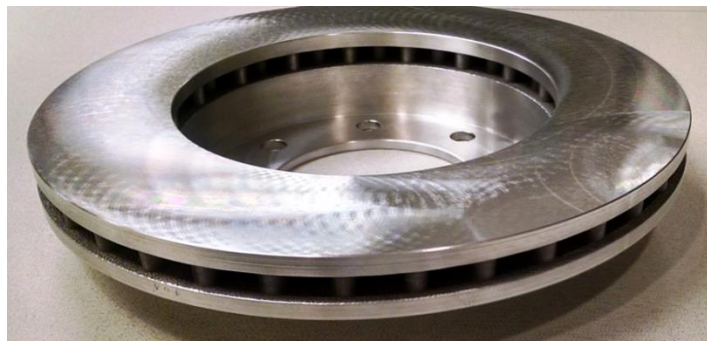


Figure 4. Al356 Cast Brake Rotor

%wt	Mn	Al	Cr	C
Fe-Mn1	25	6	4	-
Fe-Mn2	35	4	2	0.2
Fe-Mn3	25	2	2	0.1
Fe-Mn4	35	4	2	0.1

Table 1. Fe-Mn Alloy Compositions

Material	C	Cr	Ni	Mo	Si	Mn	N	Nb	V	Hardness
Nitronic 50	0.017 max	(21-25)	(11-14)	(2-3.5)	1 max	(5-6)	(0.35-0.5)	0.3	(0.15-0.35)	(C28)
Nitronic 60	0.1	(16-18)	(8-9)	-	(3.5-4.5)	(7-9)	(0.08-0.18)	-	-	(B98)

Table 2. Composition of Nitronic 50 and Nitronic 60

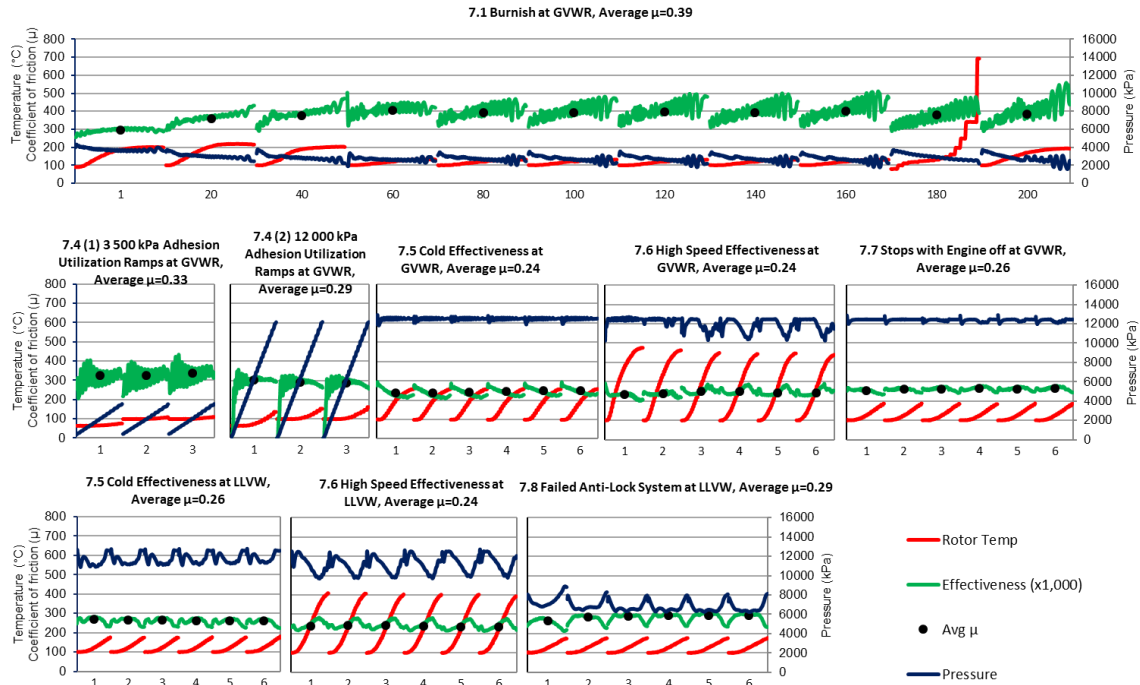


Figure 1. FMVSS test results of the coated brake rotor during various braking cycles

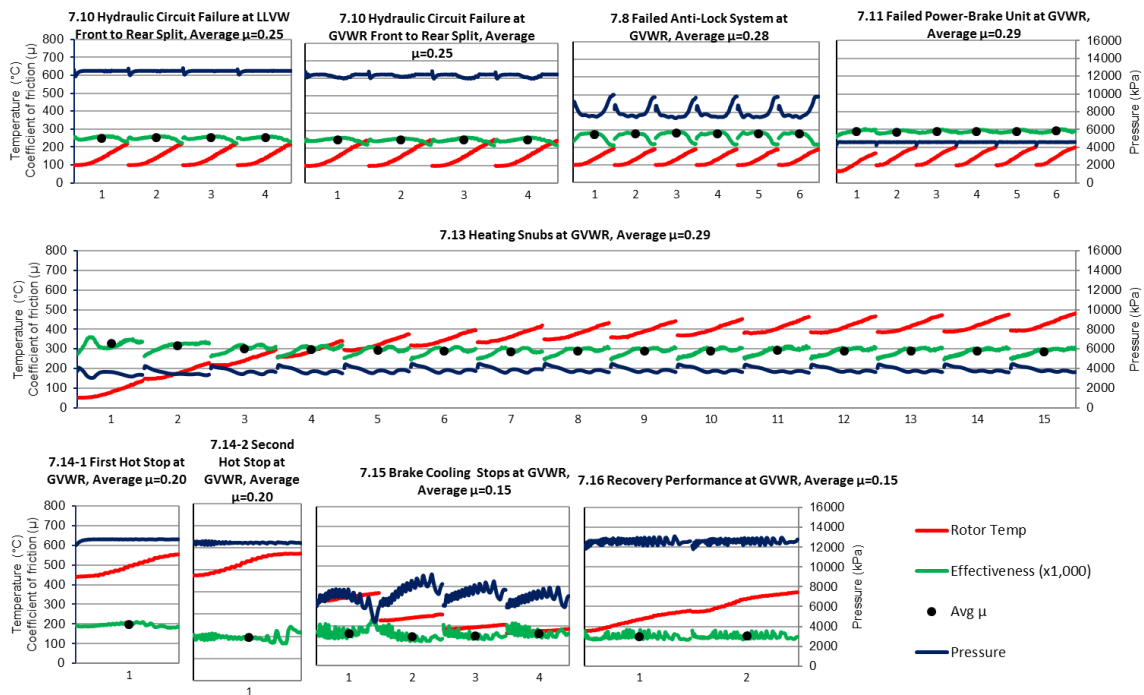


Figure 2. FMVSS test results of the coated brake rotor during various braking cycles



Figure 3. Coated aluminum rotor- Inboard side (L) and Outboard side(R)

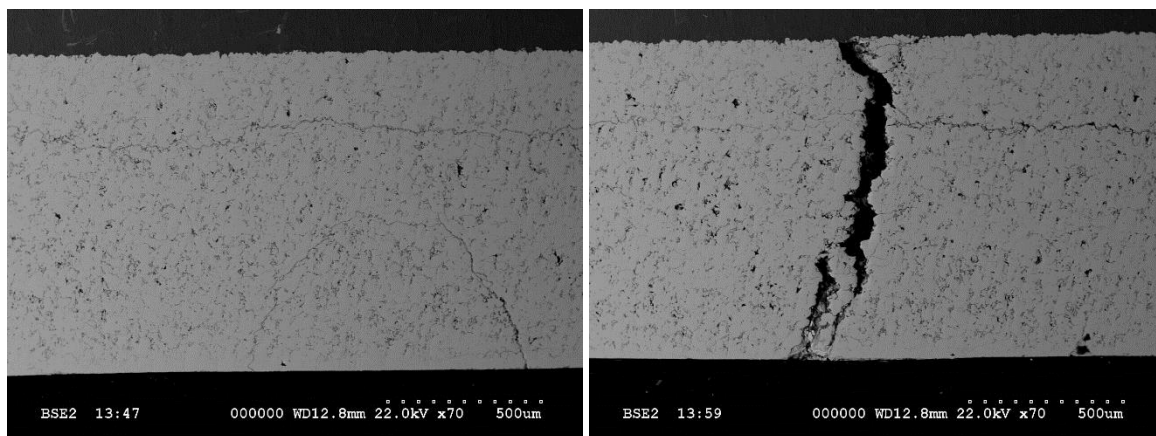


Figure 4. BSE images of rotor cross-section on Inboard side (L) and Outboard side(R)

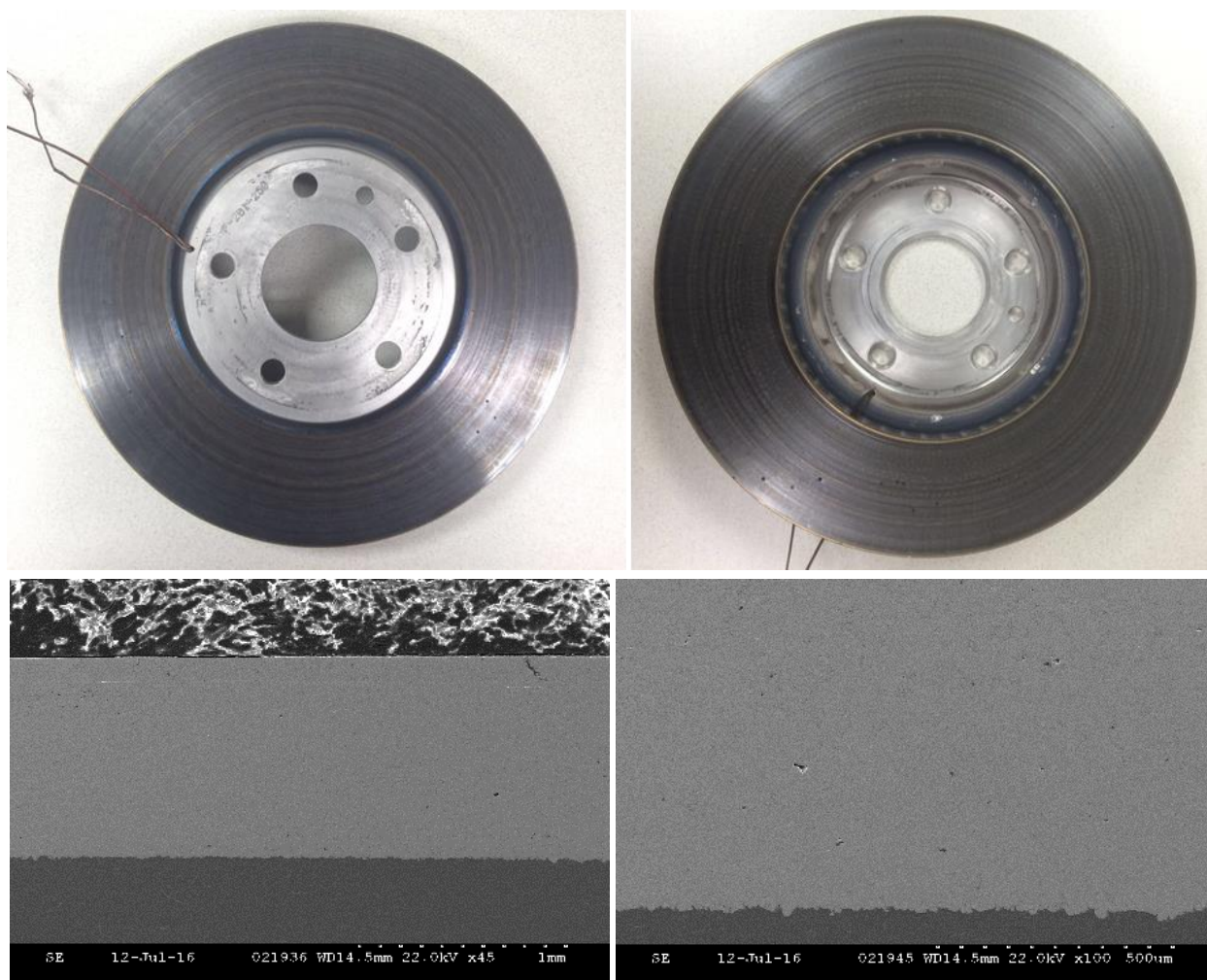


Figure 5. Previous results of coated aluminum front rotors on passenger car (4dr sedan) test platform

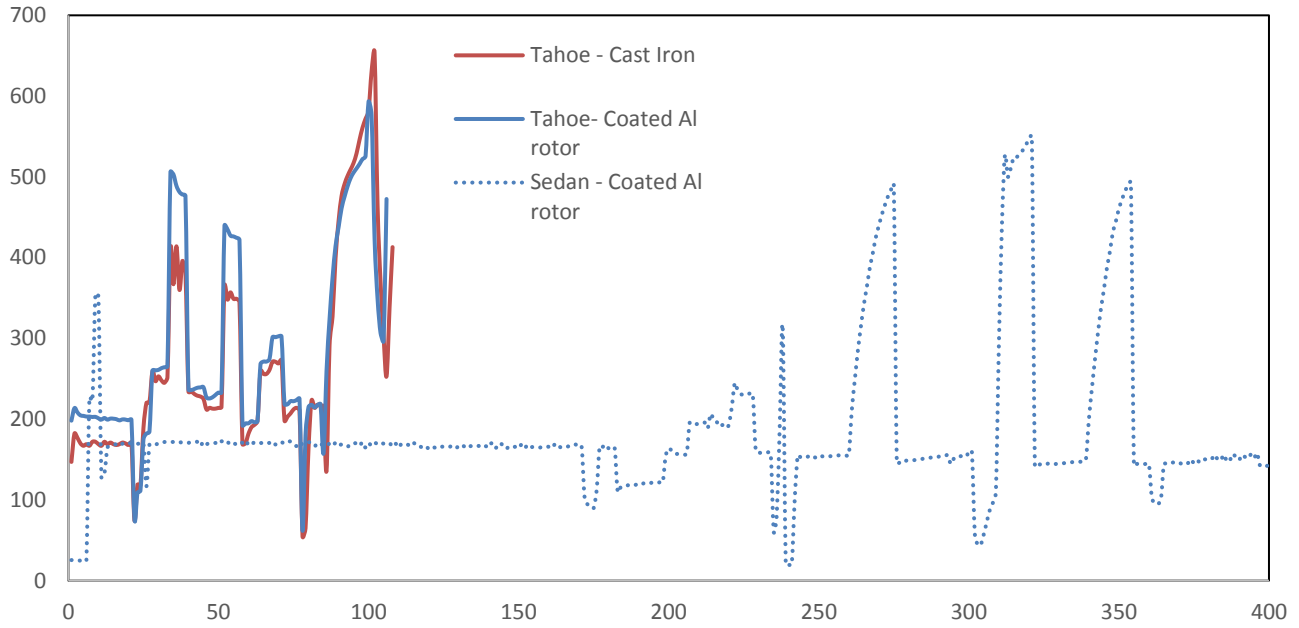


Figure 6. Recorded surface temperatures from various rotor during brake dyno-tests

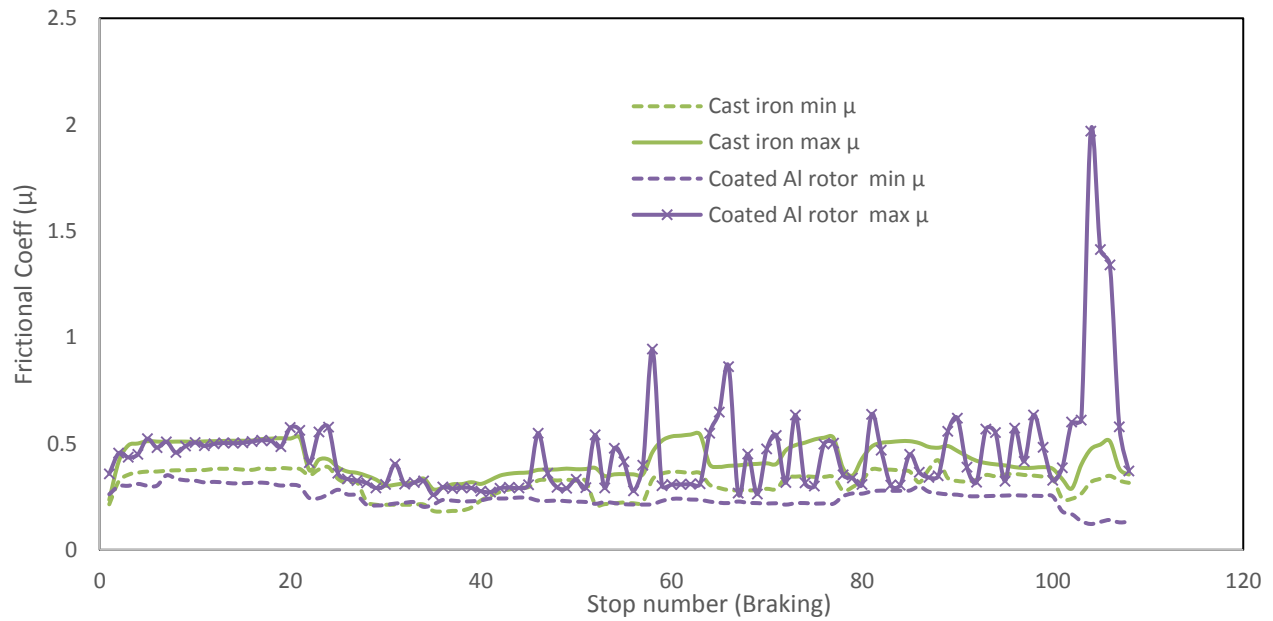


Figure 7. Coefficient of friction measured during various stops for cast iron and coated al rotors under identical tests.

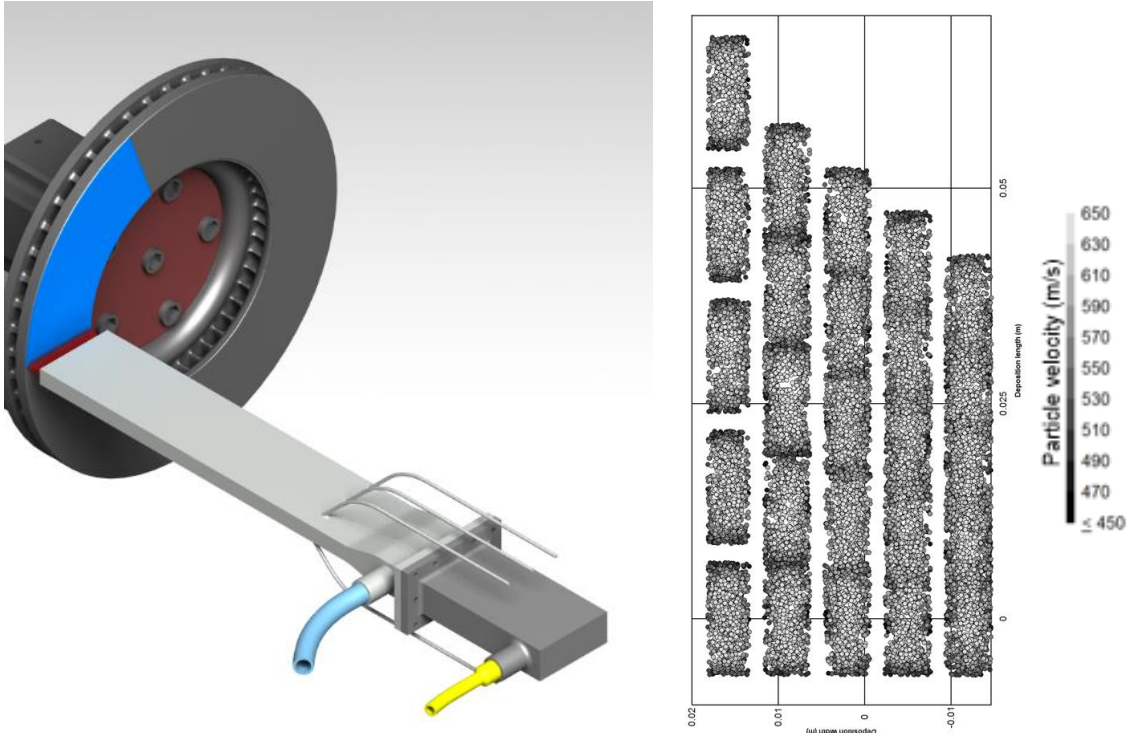


Figure 8. Wide area cold spray deposition using multiple nozzle apparatus. CAD model of deposition on rotor (L) CFD simulated particle distribution map with different nozzle overlapping segments (R)

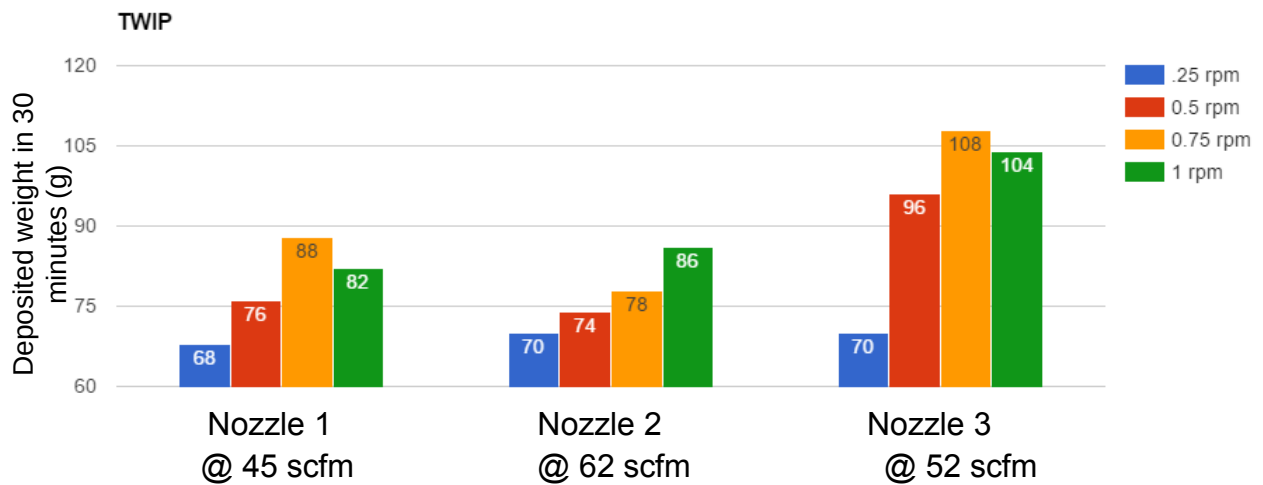


Figure 9. Deposited weights from three nozzles with different expansion ratios at different nozzle traverse velocities. SCFM (standard cubic feet per minute) indicates the nitrogen consumption rates by these nozzles.

AVPTA Technology Focus Area 2: Lightweight Structures & Materials

Multi-Material Joining (MMJ) Bolted Composite Joint Strength and Fatigue

**TARDEC POC: Bernard Sia, TARDEC
Bridging Team**

**Principal Investigator(s):
Mr. Riley Woodham, Seemann
Composites**

**Mr. Ted Campbell, Material Sciences
Corporation**

Project Start: FY11

Estimated Completion: Q4FY17

Objective(s):

- Assess how an applied load is distributed between a metallic (17-4PH stainless steel) component and intermediate modulus carbon fiber reinforced composite component joined by a series of bolts.
- Determine the effect of bolt hole size and bolt hole pattern on the performance of a composite component bolted to a metallic component.
- Determine the potential failure modes for joints comprised of a composite component bolted to a metallic component.

Strategic Context:

- Work directly contributes to the design and development of a mid-span hinge joint for a composite bridge being designed for potential use on a current assault bridge Program of Record. The Army's Product Manager for Bridging has shown interest in further development of this bridge to address the capability of military bridges to accommodate the growing weights of military vehicles such as the Abrams tank.
- Knowledge gained from this work can also be applied in other applications where stainless steel is bolted to an intermediate-modulus carbon fiber composite.

Accomplishments:

- Durability testing was completed on a modular composite bridge system previously manufactured by Seemann Composites. This provided the team with more representative dynamic factors which can be used to scale up the test loads for future hinge joint testing

- Modifications to the bridge's center hinge joint have been made to account for a heavier load requirement, and these modifications have been implemented into a new center joint test specimen.
- Coupon level corrosion testing was started.

Introduction:

The Composite Assault Bridge is a composite bridge being designed for potential use on a future Product Manager Bridging assault bridge Program of Record. One of its design elements is a mid-span joint consisting of a stainless steel hinge bolted to an intermediate modulus carbon fiber composite tension rail. The bridge's mid-span sees the highest amount of load during bridge crossing, making it the most critical component of the structure and a candidate for risk reduction. Unknowns exist with respect to how load is actually distributed between the metal and composite when connected using bolts, as well as the failure modes which may result. To resolve these unknowns, a test program was started to assess the behavior of joints comprised of intermediate modulus carbon fiber composite components bolted to stainless steel components.

Approach:

In lieu of building a full scale structure, it was decided to exercise the critical behavior of the joint through component testing utilizing associated fixturing. Figures 1-2 shows the test article design and its derivation from the full Composite Assault Bridge design. The test article consists of a stainless steel hinge fitting bolted to an intermediate modulus carbon fiber composite tension rail. These components are then placed into a steel box used to approximate the joint's boundary conditions in the overall bridge structure. Based off of the results of Test 1 in April 2013, a simulated bulkhead was added to the steel box in October 2013 to provide additional resistance to vertical loads. Figure 3 shows the test specimen inside of the test box with the simulated bulkhead installed.

A finite element model was run to simulate the test results prior to each test. To run the model, assumptions were made with respect to the following aspects of the specimen:

- Fit of the tension rail in the slotted fitting and associated friction
- Fit of bolts in normal prep holes and minimal torque
- Fit of pins in multi-lug hole and associated friction
- Geometric variations within practical tolerances
- Clearance of side walls away from the box structure and of assembled test specimen from steel box bottom plate/ rails (areas where bearing on steel is possible)
- Clamp up forces at minimum torque.

The model also included displacements which were imposed to test frame interfaces. Figure 4 shows the full test specimen placed onto a 3000-kip Southwark-Emery universal testing machine at the University of Illinois Urbana-Champaign's Talbot Laboratory. The steel box attached to the testing machine through the use of a pair of loading tangs and a link adapter

which were originally designed for the Advanced Modular Composite Bridge (AMCB) program, a previously completed program performed by Seemann Composites.

The test machine applies an axial tension load to the test article, and the test box reacts this load to the test specimen through a double shear, bolted connection. Within the test box, the test specimen is oriented at an angle of approximately 4 degrees with respect to the pull load to more accurately simulate the loads seen in the full bridge. This orientation also introduces an out-of-plane load to the specimen.

Each test consisted of seven test runs performed at the following load levels:

- Run 1: Up to 70 kips for System Checkout
- Run 2: 50% design load (175 kips)
- Run 3: 100% design load (350 kips)
- Run 4: 150% design load
- Run 5: 180% design load
- Run 6: 200% design load
- Run 7: Load specimen to failure

Visual inspections of the specimen were performed after each run. Cracking and other audible events were also listened for throughout testing. Strain, load and displacement were measured and recorded for each test.

Results and Discussion:

A contract (Contract # W56HZV-15-C-0225) was awarded to Seemann Composites on 25 September 2015 for the development of a composite assault bridge. Included in the contract is the following work being performed in support of the AVPTA project:

- Testing of three full-scale center hinge assemblies, consisting of a composite bolt bearing and by-pass test article and metallic hinge, under compression and shear loading. Each full-scale center hinge assembly shall incorporate a different bolt hole size and pattern to evaluate the effect of varying bolt hole sizes and patterns on the structural performance of the hinge.
- Testing of composite/ metallic coupons to assess the behavior of the dissimilar material combination in a corrosive environment

At the beginning of the fiscal year, work on the contract focused on supporting durability testing of the AMCB at Aberdeen Test Center. The AMCB, which was manufactured by Seemann Composites in a previous effort, is a 5 module bridge with joints manufactured primarily out of carbon fiber composites. The purpose of this test was to obtain a better understanding of the fatigue performance of composite joints and composite bridge structures, as well as the dynamic factors associated with vehicle crossings over a composite bridge. This information is very important for the future development of the center hinge joint and the overall bridge. Durability testing was performed from 17 November 2015 through 28 April 2016, and

consisted of both live vehicle crossings over the 3-, 4-, and 5-module configurations of the bridge using a Palletized Load System truck and modified M60 tank and simulated vehicle crossings on the 5-module bridge configuration. Figure 5 shows a fully loaded Palletized Load System truck crossing over the 4-module bridge. Overall, the AMCB withstood a total of 356 live crossings and 30,052 simulated crossings representative of a Palletized Load System and modified M60 tank. Due to lack of funding, the bridge was not tested to failure. While some damage was observed, none of the damage was severe enough to render the bridge non-mission capable. The AMCB exceeded the 20,000 crossing service life specified for the bridge, thus demonstrating the capability of composite bridge structures to perform well under fatigue. The test also indicated that exposure to environmental effects prior to and during testing had little to no impact on the bridge's structural behavior. The bridge had been stored outside in crates for a number of years prior to being tested, and all testing was performed outside, resulting in exposure to a variety of environmental effects. From the durability test, the team was able to derive impact factors and braking factors which can be applied to this project as well as the overall development of the bridge.

Upon completion of the durability test, focus shifted to development of the center joint for a new load requirement of Military Load Class 120. Previous testing and work on the joint had been performed at Military Load Class (MLC) 85. The load requirement was changed to ensure the bridge would be able to support the increasing weight of the Abrams tank. Table 1 provides the characteristics for a hypothetical Military Load Class 85 tank, calculated through interpolation of the hypothetical design vehicles published in NATO Standardization Agreement (STANAG) 2021, and the hypothetical Military Load Class 120 tank, as published in NATO STANAG 2021. From this developmental work and lessons learned from previous testing of the center joint, a number of changes have been made and scaled down for implementation onto an MLC 85 test article, of similar design to that shown in Figure 3, which had been built in 2014, but never tested. This modified MLC 85 test article will be used for the first center joint test being performed under this contract. Fabrication of the modified MLC 85 test article was completed in October 2016, and testing is scheduled to begin in December 2016. Future testing performed on the joint will be performed using the full scale MLC 120 design and MLC 120 loads.

Work also began to investigate the potential galvanic corrosion issues that may result from the joining of the carbon fiber reinforced polymer composite to a 17-4PH stainless steel plate using superalloy A286 fasteners. These materials are representative of the materials being used for the center joint of the bridge. A total of 51 samples are being tested as part of this investigation, consisting of the following three sample types:

- Type I – Bolt Plate (5 total)
- Type II – Flat Gap Coupon Assembly (40 total)
- Type III – Glass Veil Coupon Assembly (6 total)

Figures 6-8 show an illustration of each sample type. Type I samples are being tested in accordance with ASTM G71, while Type II and III samples are being tested in accordance with GMW14872. 120 cycles are being performed for all sample types. Testing of the samples began in September 2016. Type II and III testing is slated for completion in late December 2016, while Type I testing will be completed in early January 2017.

Conclusions:

Based off of the work performed in FY16, the following conclusions can be made:

- Modular composite bridge structures can perform well under fatigue, withstanding a high number of crossings without losing its capability to perform its mission
- Exposure to environmental effects did not affect the ability of modular composite bridge structures to support live and simulated vehicle crossings

Future work for this project will include the following:

- Completion of coupon testing level corrosion testing and analysis of the test results
- Testing of multiple hinge test articles to further investigate the performance of the multi-material joint design and assess design changes to enable the joint to carry MLC 120 loads

Performance of sub-element level corrosion testing to measure comparative strength degradation due to material loss resulting from corrosion.

References:

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2. Test Report, MSC TFR 21607/IN44, Composite Joint Assault Bridge (CJAB) Engineering and Test Management Support, July 2016
3. Status Summary Report, MSC TPR/IN45, Galvanic Corrosion Coupon-Level Testing for CJAB Hinge Joint, September 2016
4. Status Report, Composite Joint Assault Bridge Contractor's Progress Status and Management Report for August 2016, 23 September 2016.

Figures and Tables:



Figure 1. Joint Test Specimen

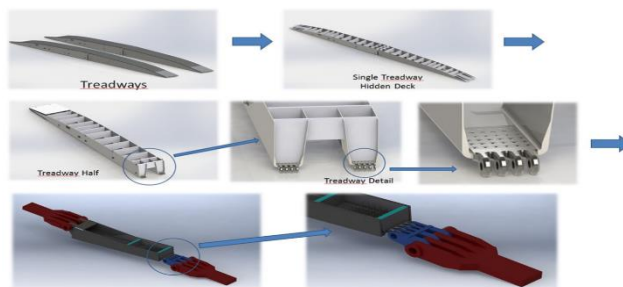


Figure 2. Derivation of Test Specimen from Bridge Design



Figure 3. Joint Test Specimen within Steel Box



Figure 4. Test Specimen Installed In Test Machine



Figure 5. Fully Loaded PLS crossing over the AMCB

	MLC 85	MLC 120
Weight (metric tons)	77.12	108.86
Track/ Ground Contact Length (m)	5.03	6.1
Outside-to-Outside Track Width (m)	3.74	4.27
Single Track Width (m)	0.87	1.02

Table 1. Comparison of MLC 85 and MLC 120 Hypothetical Tracked Vehicles

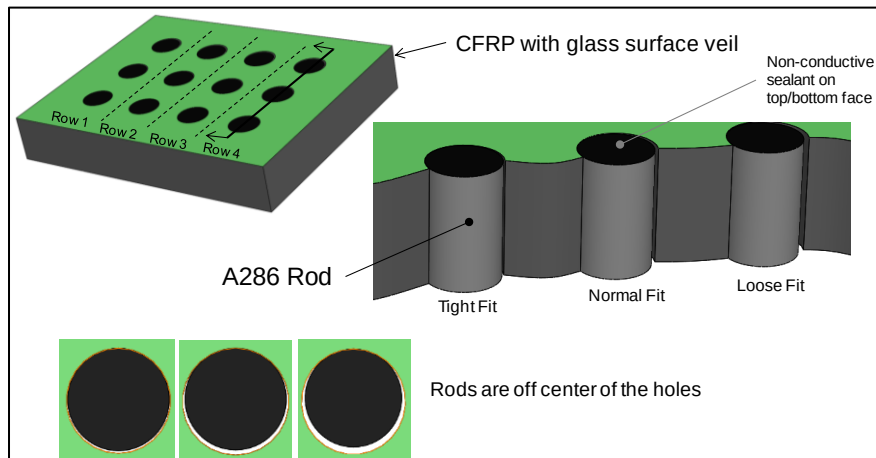


Figure 6. Type I - Bolt Plate Corrosion Test Sample

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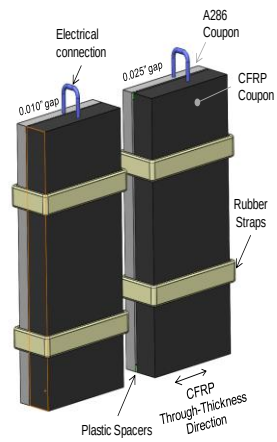


Figure 7. Type II - Flat Gap Coupon Assembly

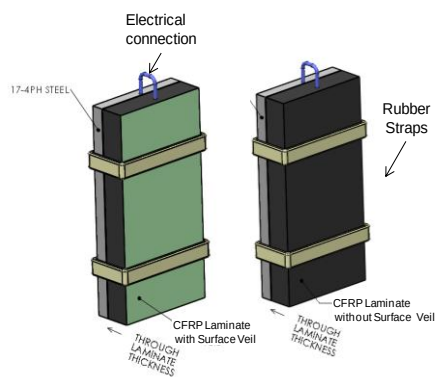


Figure 8. Type III- Glass Veil Coupon Assembly

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AVPTA Technology Focus Area 2: Lightweight Structures & Materials

Breakthrough Techniques for Dissimilar Material Joining – Collision Welding of Dissimilar Materials by Vaporizing Foil Actuator

DOE-VTO TFA Lead: Sarah Ollila
TARDEC TFA Lead: Martin McDonnell

Principal Investigators:
Dr. Glenn Daehn, Anupam Vivek, and Bert Liu

Affiliation:
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Columbus, OH 43210

Project Start: Q1FY14
Estimated Completion: Q4FY16

Objectives:

- To perform weldability screening of 15 dissimilar-metal combinations consisting of automotive Fe, Al, and/or Mg alloys
- To optimize welding parameters for select combinations
- To test corrosion performance of weld coupons, both with and without protective coating
- To gain better understanding of bonding and failure mechanisms at play
- To continue developing and maturing vaporizing foil actuator welding (VFAW) for commercialization.

Strategic Context:

- Fuel economy of vehicles can be improved by incorporating lighter, stronger materials such as high strength steel, aluminum, and magnesium.
- Vaporizing foil actuator welding (VFAW) is investigated in this work as a promising technology for joining these very dissimilar metals that are difficult to join by conventional fusion-based welding.
- Factors being evaluated include the number of alloy combinations that can be welded, weld strength, weld microstructure, and corrosion performance.

Accomplishments:

- Weld samples were studied using advanced microscopy techniques: transmission electron microscopy (TEM) and transmission Kikuchi diffraction (TKD).
- A “strong-bond” region of an AA6111-T4/DP980 weld sample was characterized by TEM. Its features match well with what was previously hypothesized about strong impact welds:
- Free of large or continuous IMC phases.
- Continuously bonded between two base metals with little diffused region in between.
- Strengthened by grain refinement.
- Reinforced by mechanical interlocking of interfacial waves (even micron-scale wave-like features).
- A list of practical considerations for actual deployment of VFAW was developed.

Introduction:

The objective of this project is to use vaporizing foil actuator welding (VFAW) to create welds between pairs of two out of three alloy systems which are relevant to commercial and military vehicles: magnesium, aluminum and steel. The ability to weld these dissimilar metals effectively can be a great enabling factor in creating lighter vehicles and improving fuel economy.

In foregoing quarters of this project, 19 such combinations were screened for weldability. Optimal welding parameters were identified for 4 of the combinations. Very strong welds were obtained for 8 of the combinations where either the peel strength exceeded 30 N/mm or the lap-shear strength exceeded the strength of a base material. 7 material pairs were subject to a 30-day-long salt-spray corrosion test, and 5 coated Al/Fe pairs retained >80% of their strengths at the end of the test.

This report features the work done in the final quarter of this project. The bonding mechanism of VFAW was investigated more deeply by advanced microscopy. Previously, AA6111-T4/DP980 samples were mechanically tested in both peel and lap-shear configurations. While a majority of samples failed in the parent aluminum during lap shear testing at an approximate load of 4000 N, one of the samples failed along the weld interface at 3500 N. The peel strength of the same weld was found to be 16 N/mm. The steel sides of fractured surfaces resulting from peel as well as lap shear tests were studied under SEM. In both peel and lap-shear cases, some areas of ductile fracture were found, whereas most of their surrounding areas exhibited features of brittle fracture (Figure 1). This somewhat corresponds with previous observation of the weld cross section, where both intermetallic compound (IMC) -ridden and IMC-free areas were found along the weld interface. The former is expected to be brittle, and the latter to be strong and tough. It is likely that the area on the fracture surface which had experienced ductile fracture corresponds with the latter type of weld interface, which is expected to be strong and tough. It is then of great interest to study the characteristics of the Al/Fe bond specifically in this area. This would allow for determination of the structure of a good weld interface with much greater confidence than before.

In the ductile-fracture areas, aluminum was found to be torn out of the bulk aluminum and transferred to the steel side. In other words, the Al/Fe bonds in these areas were stronger than the base aluminum, such that failure was forced to take place through the base aluminum rather than through the Al/Fe weld interface. These were then assumed to be areas of strong Al/Fe bonds.

Such areas were found in both lap-shear and peel fracture surfaces, but there was still distinction between the two. In lap-shear samples, such areas exhibited features of shear failure, whereas those in the peel samples often exhibited micro-void-coalescence-type tensile fracture surfaces. It is known that ductile tensile fracture requires higher stresses than ductile shear fracture, so areas where ductile tensile fracture (indicated by micro-void coalescence) was found were of particular interest in this study. Therefore, the peel sample, where the ductile fracture surface was found, was selected for further for microscopy study by TEM.

Approach:

A single ductile-fracture region in the peel sample was selected using an SEM equipped with a silicon drift EDS detector. EDS (energy dispersive X-ray spectroscopy) was used to confirm that this area indeed consisted of aluminum. Sample extraction was performed on an FEI Nova™ DualBeam FIB equipped with an Omniprobe™ in situ lift out probe and platinum deposition system. Once the region of interest was located, a platinum layer 1.5 μm thick was deposited to preserve the fracture surface during high current trenching steps. Trenching and extraction were done using standard in situ techniques, although trench size was increased to account for line of sight issues resulting from the irregular surface. The resulting slab was then attached to a copper Omniprobe grid and the bulk of material removed at an incidence angle of $\pm 3^\circ$ at 30 keV. Final thinning was done using 5 keV cleaning cross sections at $\pm 5^\circ$ until the sample reached electron transparency.

Characterization was performed using an FEI Image Corrected Titan3™ G2 60-300 S/TEM system equipped with a quad-silicon drift Super-X EDS detector. Imaging was done in both HAADF-STEM and corrected HR-TEM. Chemical maps were collected for an hour at a count rate of 16 kcps.

Results and Discussion:

Microscopic wavy features were observed as shown in Figure 2. Some areas along the interface had IMCs and some areas did not. These microscopic wavy features (less than 1 micron in height) resemble the mesoscopic wavy features (some 30 microns in height) often observed in optical microscopy, but are on a much smaller scale. These resemble fractal-like patterns in Kelvin-Helmholtz instability, where self-similar features can be found at different length scales (Figure 2(c)). An EDS line scan across an IMC-free interface showed a very sharp transition between Al and Fe.

Most of the interface is covered with a very thin layer of Al-Fe intermetallic compounds (IMC) of types FeAl, Fe₃Al, Fe₂Al₅, and FeAl₃. The thickness of the IMC layer ranged from 0 nm to 100 nm (Figure 2(a-b)). This indicates that very little diffusion or mechanical mixing occurred.

Within 2 microns of the interface, the grains on both sides of the interface are very refined, with some grains being as small as 50 nanometers (Figure 3). XRD revealed that the weld interface is fully crystalline, as shown in Figure 4. A few other researchers have reported amorphous phases at Al/Fe impact welded interfaces, but we did not observe any such phases.

Conclusions:

The findings validate the hypothesis that the interface of a strong impact weld is free of large or continuous IMC phases, continuously bonded between two base metals with little diffused region in between, strengthened by grain refinement, and reinforced by mechanical interlocking of waves (now we know that waves occur on both meso- and microscopic levels).

Acknowledgements:

The TEM work was done in collaboration with Dr. Michael Presley of the Center for Accelerated Maturation of Materials (Camm) at the OSU Center for Advanced Microscopy and Analysis (CEMAS).

References:

None

Figures and Tables:

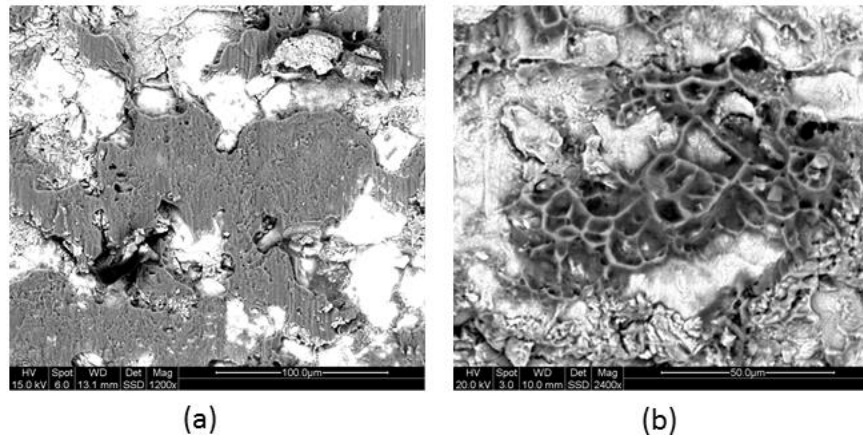


Figure 1. Steel side of ductile fracture surfaces of AA6111-T4/DP980 from (a) lap-shear mechanical testing and (b) peel mechanical testing. Darker areas represent aluminum.

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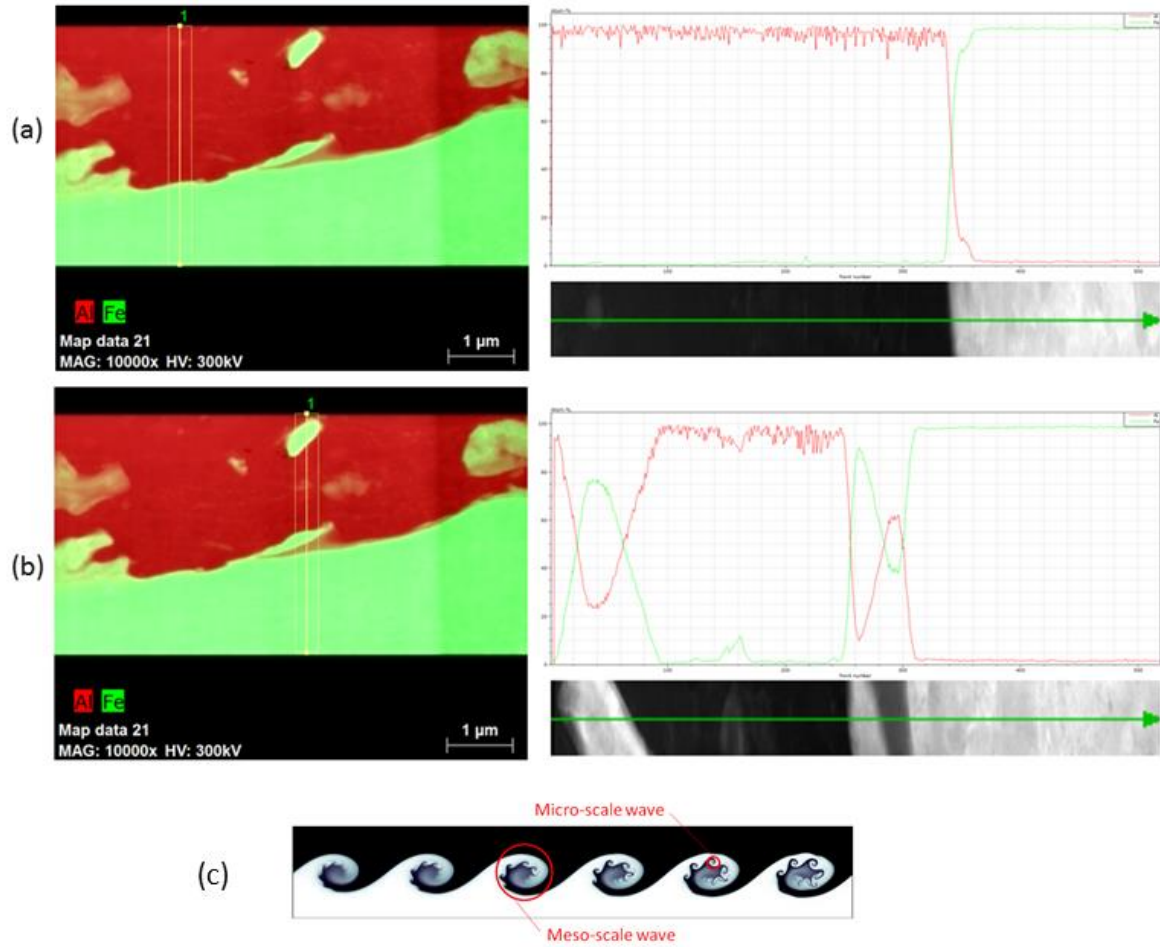


Figure 2. (a) Microscopic wavy features at the weld interface and EDS line scan across an IMC-free area of the weld interface, (b) EDS line scan across an IMC layer, (c) Kelvin-Helmholtz instability waves with self-similar waves on different scales (http://oatao.univ-toulouse.fr/606/1/Joly_606.pdf)

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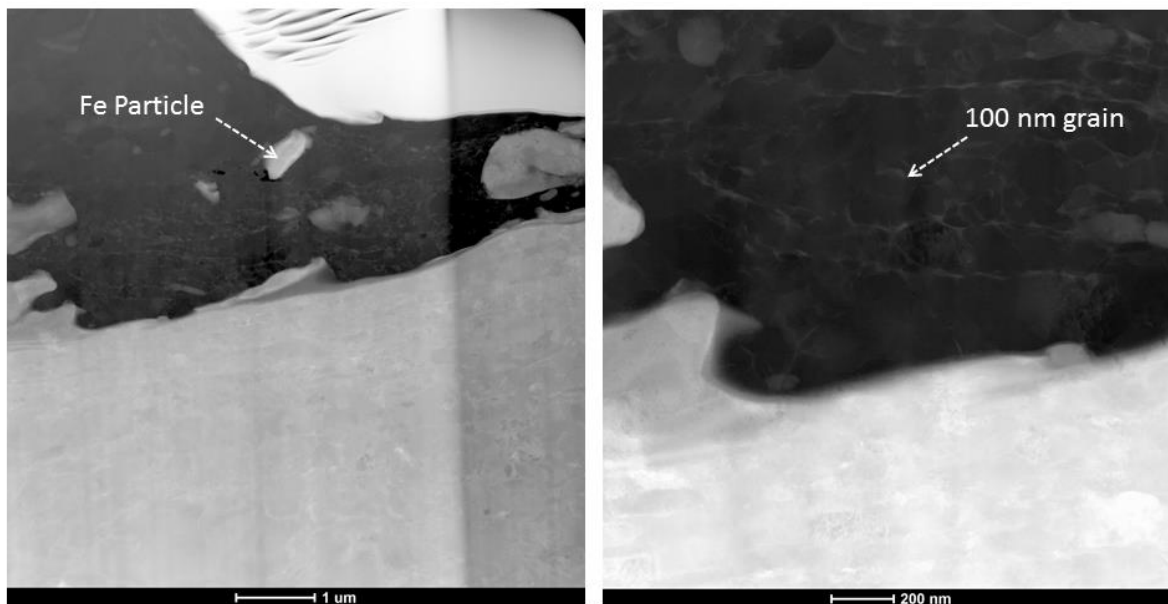


Figure 3. Highly refined grains near the interface

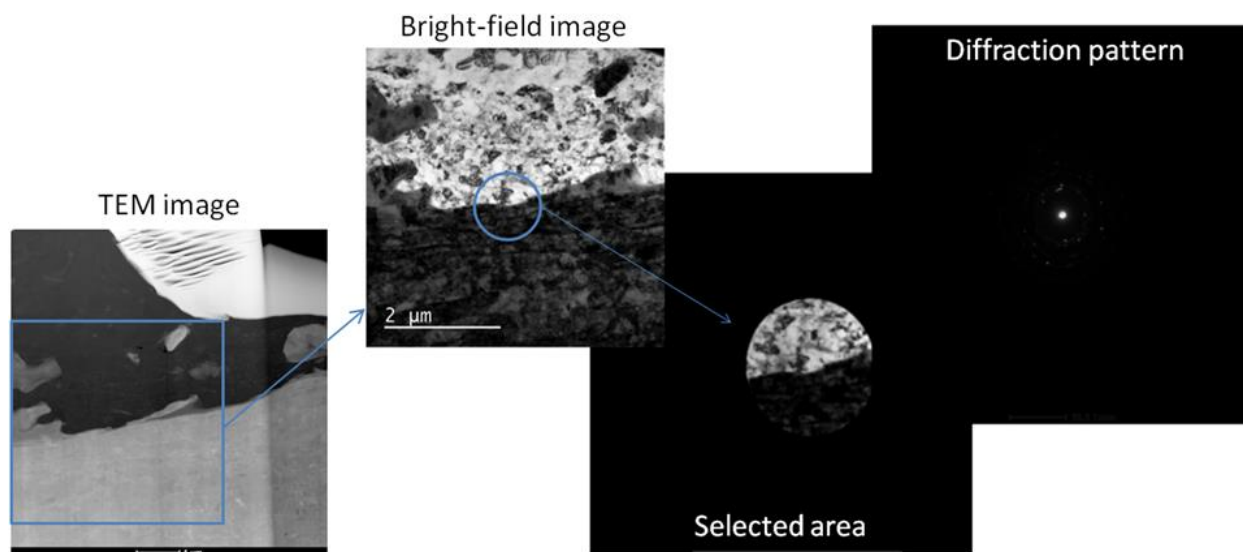


Figure 4. TEM bright field imaging and diffraction showing crystalline nature of the interface

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AVPTA Technology Focus Area 2: Lightweight Structures & Materials

Breakthrough Techniques for Dissimilar Material Joining – Upset Protrusion Joining Techniques for Joining Dissimilar Metals

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Start: Q1FY14
Projected Completion: Q4FY16

Objective:

- To develop and demonstrate a robust, cost effective, and versatile joining technique, known as Upset Protrusion Joining (UPJ), for joining challenging dissimilar metal combinations, especially those where one of the metals is a die cast magnesium (Mg) component.

Strategic Context:

- The project goal is to join magnesium castings to resin composite structures. The technology and research methodology will be used to develop similar processes for steel or aluminum castings.
- The technology supports the TARDEC Strategy enabling new capability in cost and technically effective joining of metals and composites.
- Follow-on activities may include further AVPTA interest to investigate increasing joint strength, reducing cost and/or developing foils for other casting materials.
- TARDEC-specific follow-on will depend upon project success.
- FCA, a U.S. automotive manufacturer, is leading this project. Since two of the key obstacles preventing more widespread use of light metals in high volume automotive applications are lack of robust joining techniques (especially for dissimilar metal joining) and susceptibility to galvanic corrosion, successful completion of this project will provide a key enabler to high volume application of lightweight materials, allowing FCA (and

ultimately other manufacturers) to accelerate the development of new lightweight vehicle designs that utilize multiple lightweight materials in order to aggressively reduce mass on future vehicle programs.

Accomplishments:

- Completed accelerated corrosion exposure of all 350 round boss UPJ joints per the ASTM G85-A2 (Acidified Salt Fog Testing) schedule. 218 samples successfully completed the prescribed 12-wk corrosion evaluation.
- Continued and completed post corrosion testing of 7-mm and 8-mm round boss UPJ joints. Most of the results for 8-mm round boss UPJ Mg to steel and Mg to Al joint corrosion tests were reported previously in the FY16 Annual Report.
- Continued coating activities to support production of coated round boss UCR assemblies for testing and evaluation.
- Completed production of all 384 round boss UCR assemblies as well as pre-corrosion structural/mechanical testing and evaluation of 180 assemblies, and initiated and completed accelerated corrosion evaluation of 204 assemblies per the ASTM G85-A2 (Acidified Salt Fog Testing) schedule.
- Completed post-corrosion structural/mechanical testing and evaluation of all 204 round boss UCR assemblies after exposure to the ASTM G85-A2 (Acidified Salt Fog Testing) schedule.
- Obtained 75 steel test coupons coated with the military spec CARC (Chemical Agent Resistant Coating) coating process from TARDEC to see if this coating could provide improved galvanic isolation between the steel and Mg samples compared to the previously evaluated conventional automotive coating processes.
- Obtained 40 Mg AM60B test coupons treated with Henkel's new MGC-2.0 pretreatment to determine if this coating could provide improved corrosion performance of the Mg samples compared to the previously evaluated conventional Henkel Alodine 5200 automotive pretreatment process.

Introduction:

The UPJ process, shown conceptually in Figure 1, is similar to heat staking of plastic components. The simplest form of the process uses a cast-in protrusion on a die cast component, which is aligned with a clearance hole in a mating component. An application of force and heat are used to upset forge the protrusion into a larger diameter boss that fills the clearance hole and forms a mushroom-shaped head that solidly locks the two components together.

The process was conceived primarily for joining Mg die-castings to each other and to dissimilar metals because die casting is the most common and cost effective process for producing light weight Mg components yet there has been relatively little work aimed at joining components produced from this process (other than bolting).

While alternative dissimilar metal joining processes have been investigated with varying levels of success, galvanic corrosion has consistently been demonstrated to be a key challenge. Particularly:

- Metallic bonding such as fusion or solid state welding processes, which require a clean (no coatings, or a specific coating designed to improve intermetallic bonding rather than corrosion performance) surface on both metals and does not allow for any isolation between the two metals.
- Separate fastener (rivet, bolt, etc.). Typically, separate fasteners are made of steel for high strength and low cost. However, steel fasteners promote galvanic corrosion in aluminum and aggressively promote galvanic corrosion in magnesium. This galvanic activity is even worse if one of the two light metals is joined to a steel component. Additionally, any coatings on the steel fasteners intended for corrosion protection tend to get damaged during the installation process and the fasteners also tend to damage any coatings on the components being joined, thus rendering any preliminary coatings to be useless since the isolation has been broken, or even magnifying the galvanic attack on the anode if a small defect is created in the coating of the anode. Figure 2 shows an example of this magnified galvanic attack when a coated steel screw is driven into a coated magnesium component and then exposed to a corrosive environment.

By contrast, the UPJ process relies on a robust mechanical joint rather than intermetallic bonding, so the more cathodic material can be coated prior to joining to protect against galvanic attack on the more anodic material. Additionally, since the UPJ protrusion is going through a hole that can be pre-drilled or pre-punched prior to coating, the UPJ process is much less likely to damage the coating when the joint is being made. Furthermore, since there is no additional cathodic material (such as a steel fastener) used to create the joint, there is no joining induced galvanic activity beyond that between the two parent materials.

Approach:

The project technical approach is summarized as follows:

- Establish *benchmark* performance of magnesium to aluminum joints produced through SPR, a currently available commercial process, *for comparison purposes only*.
- Obtain additional knowledge and understanding of thermo-mechanical behavior of magnesium alloys through Gleeble® testing conducted in Canada at no cost to the U.S. Department of Energy (DOE).
- Take advantage of knowledge that FCA has already gained on the UPJ process, as well as additional CAE forming simulations based on the knowledge gained through the Gleeble® testing, to develop optimized cast protrusion and welding electrode shapes to reduce electrical current requirements and provide more robust, repeatable forming performance for each of the joint configurations being considered.

- For each configuration (AM60B to Al6022, Al6013, and high-strength steel (HSS) in bare, pretreated, and coated conditions, and round and oval shaped joints), produce tensile shear and cross tension test coupons, and send select assemblies back for additional coating layer prior to actual start of mechanical/structural and corrosion evaluations.
- Subject a substantial number of samples (five of each configuration) to initial mechanical/structural tests as described above.
- Subject a substantial number of samples to FCA's accelerated corrosion tests, reviewing visually every two weeks and removing three samples of each configuration at four week intervals for quasi-static testing.
- Finally, at the end of the 12-week accelerated corrosion exposure, subject select configurations to fatigue and impact testing for comparison to pre-corrosion performance.

Joint performance is validated through:

- Characterization of material microstructure in the joint region
- Characterization of joining-induced defects in the joint region
- Quasi-static tensile shear tests
- Quasi-static cross-tension tests
- Drop tower impact tests of select tensile shear and cross-tension samples
- Cyclic fatigue testing of select tensile shear and cross-tension samples
- Exposure to 12 weeks of FCA's accelerated corrosion test (ASTM G85-A2) with quasi-static lap shear failure and cross tension failure being evaluated after each 4-week increment, and fatigue testing and impact testing to be re-evaluated on select samples at the end of corrosion exposure
- Characterization of failure mechanisms for each of the mechanical tests described above.

Results and Discussion:

In FY2016, the team completed accelerated corrosion testing and post corrosion mechanical testing of all round boss UPJ joints as well as production, accelerated corrosion exposure, and post corrosion testing of all round boss UCR joints. After completion of all of this pre-defined work, the team began to investigate alternative corrosion coatings.

The sample material/coating configuration descriptions for all round boss UPJ joints discussed in this report are shown in Table 1. The configuration numbers defined in this table will be used throughout the report.

Impact Lap Shear Tension:

Test results for configurations UPJ8-2 and UPJ8-4 are shown in Figure 3 prior to corrosion testing and after 12-wks of accelerated corrosion exposure (left) and the failure mode for UPJ8-4 after corrosion is shown in Figure 3 (right). This sample failed through shearing of the protrusion. It should be noted that although there is not a substantial drop in impact performance after corrosion exposure, the data *range* for the results has increased substantially.

Impact Cross Tension:

Test results for configurations UPJ8-1, UPJ8-2, UPJ8-3, and UPJ8-5 are shown in Figure 4 prior to corrosion testing and after 12-wks of accelerated corrosion exposure. The failure modes for UPJ8-3 and UPJ8-5 after corrosion are shown in Figure 5. These samples failed through partial thickness protrusion pull-out, head of protrusion fracturing, and base of protrusion fracturing.

Lap-shear Tension Fatigue:

Results prior to corrosion and at 12-wks corrosion exposure are shown in Figure 6. It is interesting to note that for lap shear tension fatigue, the post corrosion samples (shown in purple) failed at lower levels than the pre-corrosion samples in low cycle fatigue, but not at high cycle fatigue.

Cross Tension Fatigue:

Results are shown in Figure 7. For cross tension fatigue, the post corrosion samples (again shown in purple) failed at dramatically higher levels (2-3 times higher) than the pre-corrosion samples in high cycle fatigue. This was completely unexpected, and investigation of several possible theories was unable to identify the reason for the increase.

Figure 8 shows the results of 12-wks of accelerated corrosion exposure for Bare Mg AM60B to Bare Al 6016 lap shear tension test samples. It should be noted that none of the lap shear samples separated as a result of the 12-wk corrosion test. Figure 9 shows similar results for pretreated Mg to pretreated Al joints with the powder-coating applied after assembly and Figure 10 shows results for pretreated Mg to powder-coated Al without any coating being applied after assembly. The significantly improved results for these samples compared to the 8-mm round boss samples that have been discussed in previous reports is primarily due to the different aluminum alloy. For the earlier reports, the Al coupons were Al 6013, which is a high copper content Al alloy. For the samples discussed in this report, the Al coupons are Al 6016, which is a very low copper content Al alloy. Copper is well known to be aggressive to Mg when exposed to an acidic environment, and apparently (from the previous samples) also has a very detrimental effect on the intergranular exfoliation corrosion of aluminum sheet material.

Interestingly, while none of the cross tension samples separated during the 12-wk corrosion exposure either, one sample from each coating configuration did experience substantial corrosion of the Mg coupons well away from the joint. Figure 11 shows some of the cross tension samples with damage to the Mg coupons. The reason for this is not completely clear since: (a) none of the lap shear samples experienced the same type of damage, and (b) this particular type of damage was not observed in the previous corrosion testing with the Mg to Al 6013 or Mg to steel joints. However, a likely explanation could be that water may have pooled in the areas of the trays in the corrosion chamber where those samples were positioned.

Quasi-static Lap Shear Tension:

Results for UPJ7-1, UPJ7-2, UPJ7-3, and UPJ7-4 are shown in Figure 12 prior to corrosion testing and after 4-wks, 8-wks, and 12-wks of accelerated corrosion exposure. All of these configurations incorporate a 6016 alloy which has a lower level of copper than the 6013 alloy used in the UPJ8-2, UPJ8-4, UPJ8-5, and UPJ8-6 configurations so the general level of performance degradation (especially related to exfoliation corrosion) after corrosion exposure is expected to be less, and in fact, none of these joints separated during the accelerated corrosion testing. Even the UPJ 7-1 configuration, which consists of bare Al joined to bare Mg with no pretreatments or coatings on either material remained intact throughout the full test regimen.

It should be noted that the aluminum panel in this configuration is only 1.1 mm thick so the overall strength levels in both lap shear tension testing and cross tension testing are lower than for the UPJ8-2, UPJ8-4, UPJ8-5, and UPJ8-6 configurations. The failure modes for all four configurations through 12 wks of exposure are shown in Figure 13. The failures occur consistently by deformation and tearing in the thin 1.1 mm aluminum top sheet. In this figure, the aluminum sheet is on the bottom. The reason for the overall lower level of performance of the UPJ7-1 configuration is that this particular configuration is the only configuration that was not painted. Since all of these samples failed in the aluminum panel and 6016 is a bake hardening alloy, then the increased strength of the 6016 alloy after paint baking in UPJ 7-2, UPJ7-3, and UPJ7-3 resulted in higher joint strength.

Quasi-static Cross Tension:

Results for UPJ7-1, UPJ7-2, UPJ7-3, and UPJ7-4 are shown in Figure 14 prior to corrosion testing and after 4-wks, 8-wks, and 12-wks of accelerated corrosion exposure. The failure modes for all four configurations through 12-wks of exposure are shown in Figure 15. The failure modes are primarily related to deformation in the thin 1.1 mm upper aluminum sheet, although UPJ7-3 failed by partial protrusion pull-out. In this figure, the aluminum sheet is on the bottom.

Again, as in the case of the lap-shear tension testing, due to the lower level of copper in the Al-6016 coupons vs. the Al-6013 alloys evaluated with the 8-mm round boss UPJ joints, none of the joints separated during the accelerated corrosion testing, even the UPJ 7-1 configuration, which consists of bare Al joined to bare Mg with no pretreatments or coatings on either material.

Note that unlike the lap-shear tension testing, in cross-tension testing, the UPJ7-1 configuration did not exhibit significantly lower joint strength than the other configurations. This is because in cross-tension, the joint strength is more dependent on the material stiffness than in lap-shear, so the additional strength gained through paint baking has less effect on the overall joint strength.

Impact Lap Shear Tension:

Results for UPJ7-1 and UPJ7-4 are shown in Figure 16 prior to corrosion testing and after 12-wks of accelerated corrosion exposure. The failure modes are shown in Figure 17. Similar to the quasi-static testing, the failures occur consistently by deformation and tearing in the thin 1.1 mm aluminum top sheet. In this figure, the aluminum sheet is on the bottom.

Impact Cross Tension:

Results for UPJ7-1 and UPJ7-4 are shown in Figure 18 prior to corrosion testing and after 12-wks of accelerated corrosion exposure. The failure modes are shown in Figure 19. Failures occurred by deformation in the thin 1.1 mm aluminum top sheet and by partial protrusion pull-out. In this figure, the aluminum sheet is on the bottom.

For the UCR evaluations, all of the configurations incorporated a 1.3 mm thick 6016 alloy coupon joined to either a 1.0 mm thick (UCR 1-4) or 1.4 mm thick (UCR 5-8) DP590 coupon. Because earlier evaluation of Mg to steel round boss UPJ assemblies had demonstrated that these joints would not pass the full 12-wk test with the current coating configurations, the test protocol for the UCR Al to steel joints with Mg rivets was reduced to only 6 weeks and the samples were evaluated on a weekly basis instead of a bi-weekly basis. All configurations except for the e-coated assemblies with sealed edges were tested at one week as well. The sample material/coating configuration descriptions for all round boss UCR joints discussed in this report are shown in Table 2.

Figure 20 shows close-up views of the actual joint for UCR lap shear tension configurations 1-4 prior to corrosion exposure and at 1, 2, 4, and 6-wks of exposure. In all of these views, the rivet head on the steel side is shown. Clearly, when joining Al to steel with a Mg rivet, it is imperative to provide a substantial coating on the steel, as well as sealing around the head and between the panels, and coating the assembly afterward as well, as was done for UCR-4. It should be noted that although UCR-4 displayed dramatically improved performance over UCR configurations 1-3, that 6-wks is still only about half of the desired longevity in this corrosive environment, so improved coating processes (especially for the steel) are required for joining of Al to steel with a Mg rivet.

Quasi-static Lap-shear Tension:

Results for all UCR joints are shown in Figure 21 prior to accelerated corrosion exposure, and at 1-wk, 2-wks, 4-wks, and 6-wks of exposure. All of these configurations incorporate a 1.3 mm thick 6016 alloy coupon joined to either a 1.0 mm thick (UCR 1-4) or 1.4 mm thick (UCR 5-8) DP590 coupon. Similar to the previously evaluated round boss UPJ Mg to steel assemblies, with the exception of UCR-4 and UCR-8 (the e-coated samples with sealed edges), all of the samples displayed a dramatic drop in strength over only two weeks of exposure. UCR-4 and UCR-8, however both maintained good joint strength levels even after 6-wks of exposure. Failure modes are shown in Figure 22.

Quasi-static Cross Tension:

Results for all UCR joints are shown in Figure 23 prior to accelerated corrosion exposure, and at 1-wk, 2-wks, 4-wks, and 6-wks of exposure. Similar to the lap-shear tension testing described above, with the exception of UCR-4 and UCR-8, all of the samples displayed a dramatic drop in strength over only two weeks of exposure. UCR-4 and UCR-8, however both maintained good joint strength levels even after 6-wks of exposure. Post-corrosion failure modes are shown in Figure 24. All pre-corrosion samples failed at the base of the rivet.

Impact Lap Shear Tension:

Results and failure modes for UCR-4 and UCR-8 prior to corrosion and at 1-wk, 2-wks, 4-wks, and 6-wks of accelerated corrosion exposure are shown in Figures 25 and 26 while Cross tension impact results and failure modes are shown in Figures 27 and 28.

Lap-shear Tension Fatigue:

Results prior to corrosion and after 4-wks of corrosion exposure are shown in Figure 29. Results are generally consistent with previously reported results for UPJ lap-shear tension fatigue testing although the high cycle fatigue results are higher since the actual base materials are steel and aluminum and only the rivet is magnesium. In previous UPJ lap-shear fatigue testing, many of the high cycle fatigue failures had occurred in the die cast magnesium plate. Failure modes for UCR8 lap shear tension testing are shown in Figure 30 where it can be seen that all of the pre-corrosion samples failed in the parent material of the lower 1.3 mm aluminum sheet. However, while some of the post-corrosion samples failed in the aluminum parent material, others failed in the actual rivet head.

Cross Tension Fatigue:

Results are shown in Figure 31. Again, results are generally consistent with previously reported results for UPJ cross tension fatigue testing with the exception that there is not a dramatic increase in post-corrosion high cycle fatigue vs. pre-corrosion high cycle fatigue. As can be seen in Figure 32, all of the samples failed at the base of the rivet.

The alternative CARC coating provided by TARDEC was unable to withstand the UPJ process temperatures and forces as can be seen in Figure 33. Due to the extensive coating damage in the area of the UPJ joint, no corrosion testing was conducted.

The MGC-2.0 Mg pretreatment provided by Henkel converts the outer layer of the Mg material to a ceramic. However, this coating was unable to withstand the UPJ process forces as can be seen in Figure 34(a-b) where most of the black MGC-2.0 coating flaked away from the boss in the form of a very fine powder when the UPJ force was applied prior to application of heat. However, this did not prevent the formation of a good mechanical joint as can be seen in Figure 34(c). Parts were returned to Henkel for evaluation where it was determined that even though most of the black color was gone from the boss, approximately 50-75% of

the actual coating thickness still remained. Nevertheless, subsequent corrosion testing at AET showed no improvement over the previous results with Alodine 5200 for joints where the assembly was not powder-coated post-assembly.

Conclusions:

During FY16, the team has continued evaluation of corrosion performance and post-corrosion structural/mechanical performance of 7.0 mm and 8.0 mm diameter round boss UPJ joints of Mg to Al-6013, Mg to Al-6016, and Mg to HSS DP-590 steel. While there had been substantial corrosion damage to joints produced with the uncoated Mg to Al-6013 joints and to all Mg-steel joints, the corrosion performance of the Mg to Al-6016 joints was successful even in the uncoated samples.

Also, the team produced round boss UCR Al-steel joints, and conducted pre-corrosion structural mechanical testing, corrosion testing, and post-corrosion mechanical testing of these joints. While the pre-corrosion joint performance with these joints was on par with the UPJ joints, the corrosion and post-corrosion performance posed a substantial challenge with the galvanic coupling of the three metals (Mg rivet, Al and steel plates).

Additionally, two alternative coating processes were evaluated for their performance as galvanic corrosion protection. However, neither of these alternative coating processes showed an improvement over the current state-of-the-art processes.

Overall, work in 2016 validated the ability of the UPJ and UCR processes to produce robust joints between Mg to Al, Mg to steel, and even Al to steel. Additionally, joints of Mg to Al-6016 showed good post corrosion performance as well. However, when joining Mg to Al-6013, pretreatment and coatings are absolutely necessary to obtain good corrosion performance, and Mg to steel joints will require improved coatings in order to meet corrosion performance specified in this project.

References:

None

Figures and Tables:

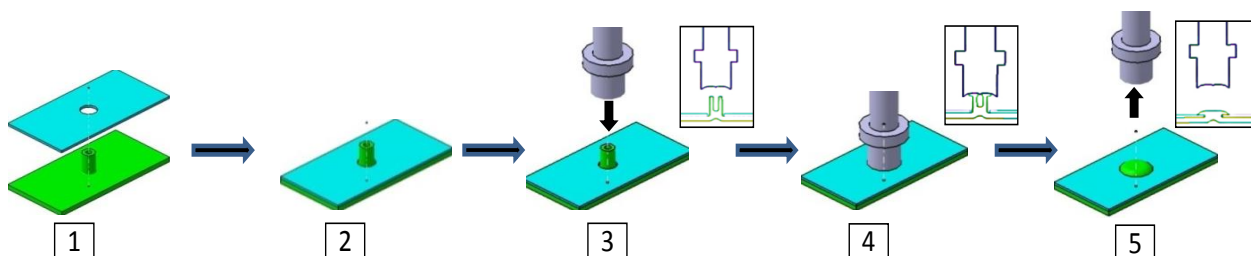


Figure 1. Initial conceptual schematic of UPJ process – assembling parts, applying heat and force, assembly complete.



Figure 2. Galvanic corrosion effects of steel screws in a magnesium component exposed to 240 hours of ASTM B117 salt spray testing.

Configuration Number	Upper Sheet			Bottom Sheet			Assembly Coating Configuration
	Material	Thickness (mm)	Coating	Material	Thickness (mm)	Coating	
UPJ7-1	Al 6016	1.1	Bare	Mg AM60B	4.0	Bare	Uncoated
UPJ7-2	Al 6016	1.1	Alodine 5200	Mg AM60B	4.0	Alodine 5200	Powdercoated
UPJ7-3	Al 6016	1.1	Powdercoated	Mg AM60B	4.0	Alodine 5200	Uncoated
UPJ7-4	Al 6016	1.1	Powdercoated	Mg AM60B	4.0	Alodine 5200	Powdercoated
UPJ8-1	HSS DP-590	2.0	Armorgalv®	Mg AM60B	4.0	Alodine 5200	Uncoated
UPJ8-2	Al 6013-T4	2.2	Bare	Mg AM60B	4.0	Bare	Uncoated
UPJ8-3	HSS DP-590	2.0	Armorgalv®	Mg AM60B	4.0	Alodine 5200	Powdercoated
UPJ8-4	Al 6013-T4	2.2	Alodine 5200	Mg AM60B	4.0	Alodine 5200	Powdercoated
UPJ8-5	Al 6013-T4	2.2	Powdercoated	Mg AM60B	4.0	Alodine 5200	Uncoated
UPJ8-6	Al 6013-T4	2.2	Powdercoated	Mg AM60B	4.0	Alodine 5200	Powdercoated

Table 1. Round Boss UPJ material and coating configurations

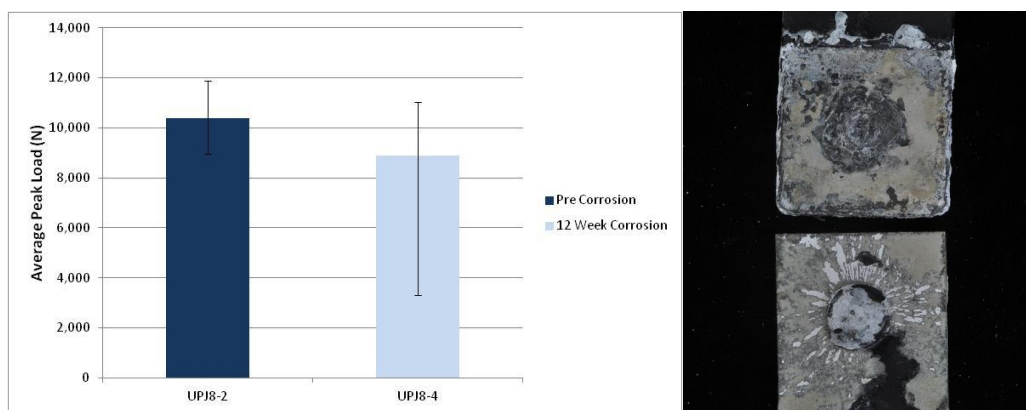


Figure 3. 8-mm round boss UPJ lap shear tension impact performance prior to corrosion testing and at 12-wks exposure (left) and failure mode (right)

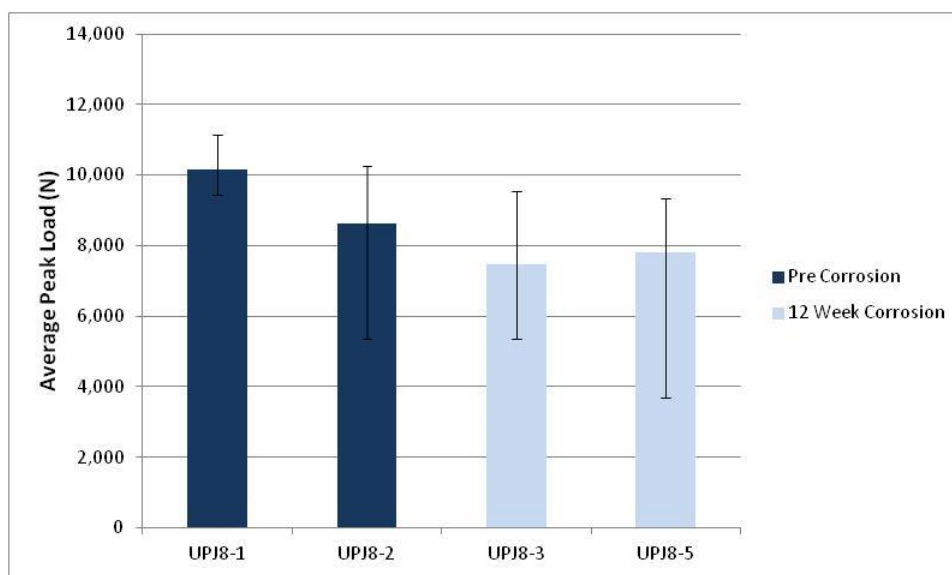


Figure 4. 8-mm round boss UPJ cross tension impact performance prior to corrosion testing and at 12-weeks exposure

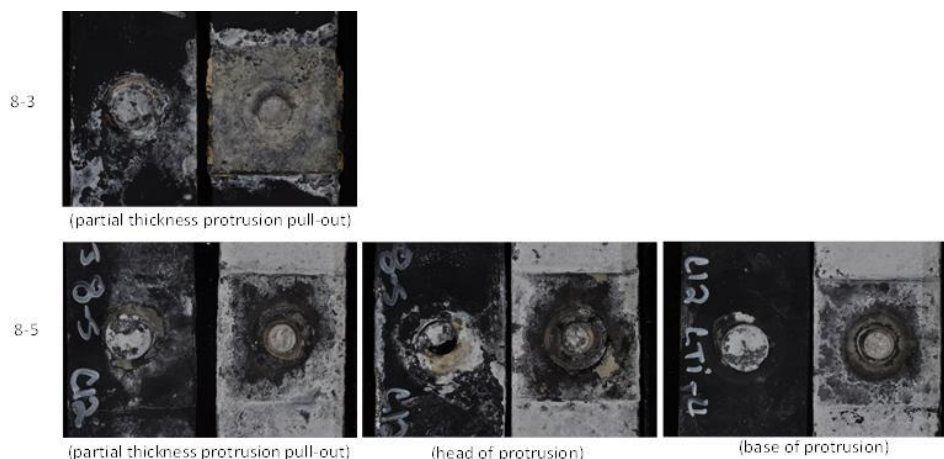


Figure 5. 8-mm round boss UPJ impact cross tension samples at 12-weeks exposure

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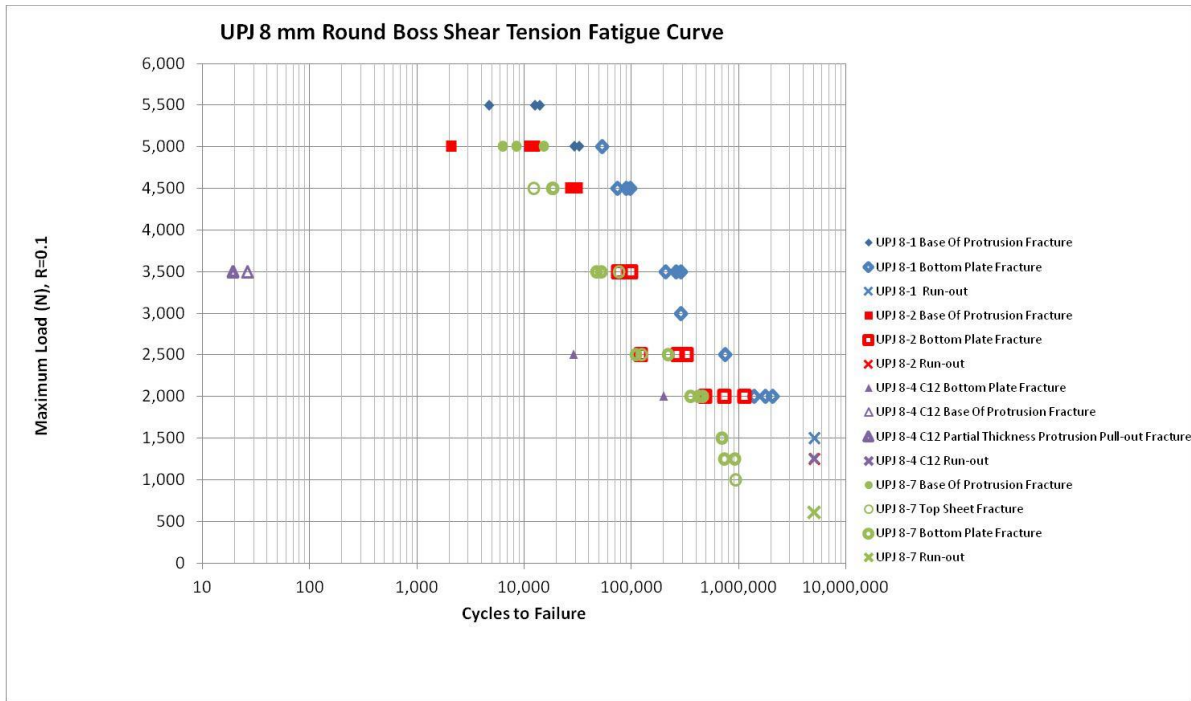


Figure 6. Comparison of 8-mm round boss UPJ lap-shear tension fatigue performance prior to corrosion testing and at 12-weeks exposure

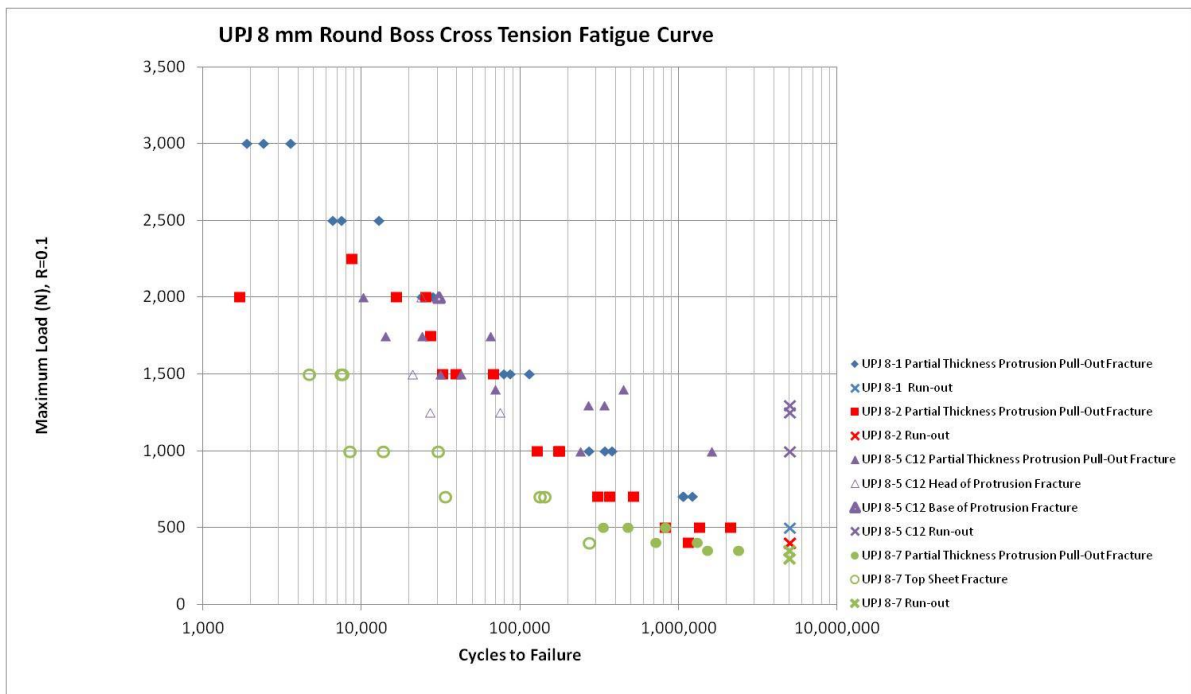


Figure 7. Comparison of 8-mm round boss UPJ cross tension performance prior to corrosion testing and at 12-weeks exposure



Figure 8. UPJ7-1 bare Mg to bare Al lap shear tension test coupons before corrosion exposure (left) and after 12-weeks of exposure (right)

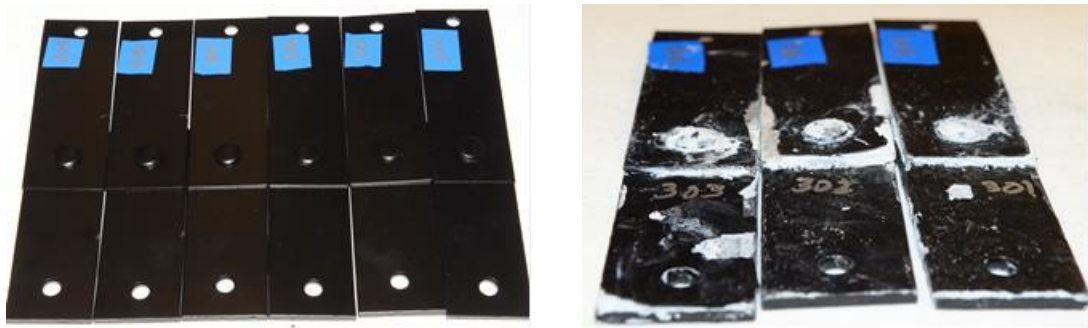


Figure 9. UPJ7-2 pretreated Mg to pretreated Al lap shear tension test coupons with coating applied after assembly, before corrosion exposure (left) and after 12-weeks of exposure (right)

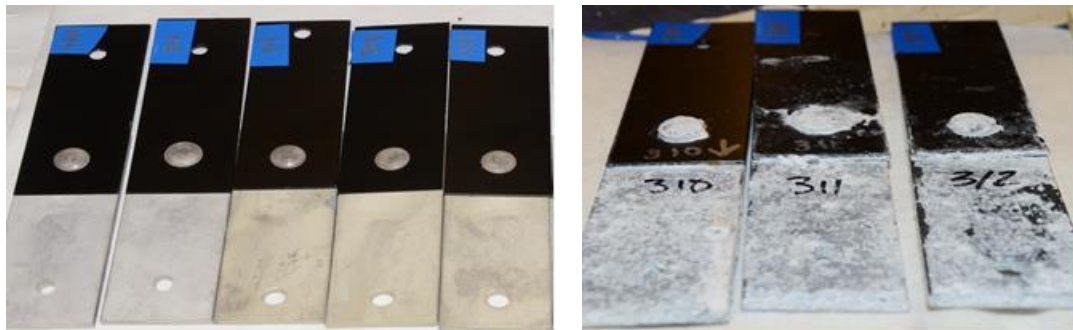


Figure 10. UPJ7-3 pretreated Mg to powder-coated Al lap shear tension test coupons, before corrosion exposure (left) and after 12-weeks of exposure (right)

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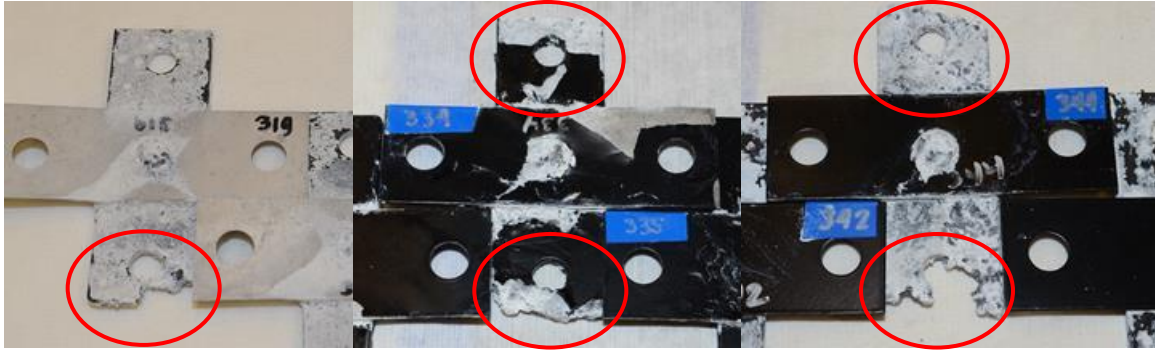


Figure 11. From left, UPJ7-1, 7-2, and 7-3 Mg to Al cross tension test coupons after 12-weeks of exposure

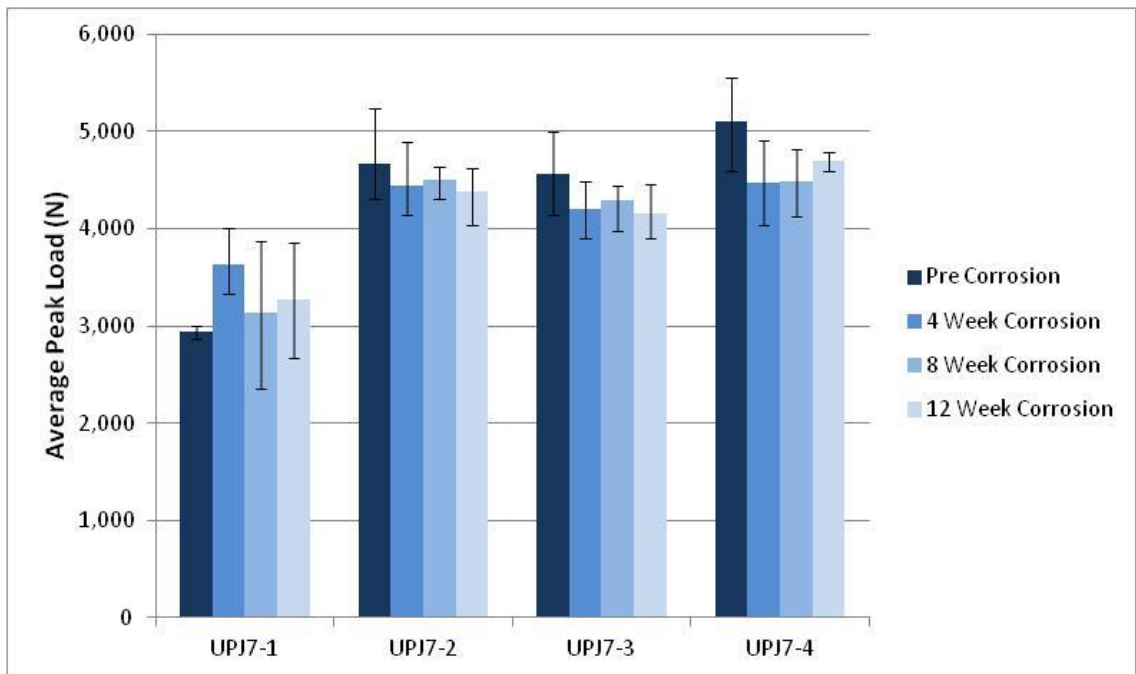


Figure 12. 7-mm round boss UPJ quasi-static lap shear tension performance prior to corrosion testing, at 4-wks, 8-wks, and 12-weeks accelerated corrosion exposure

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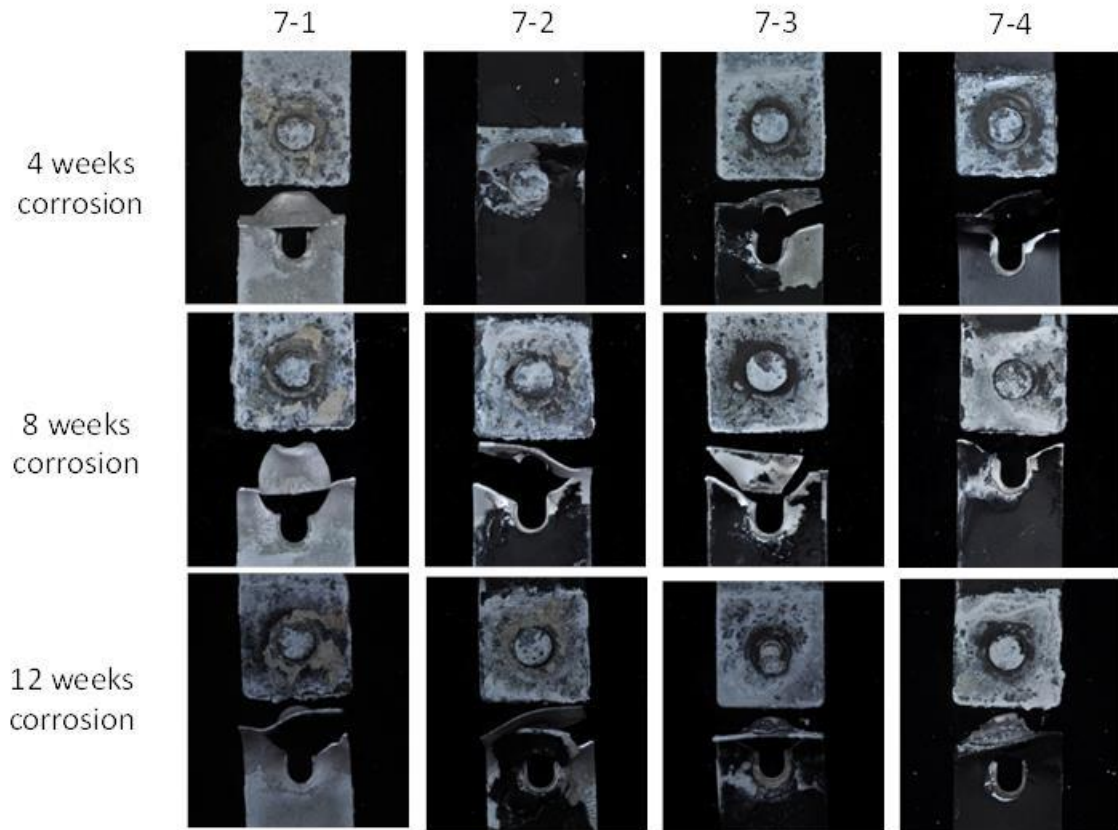


Figure 13. 7-mm round boss UPJ quasi-static lap shear tension performance failure modes after accelerated corrosion exposure

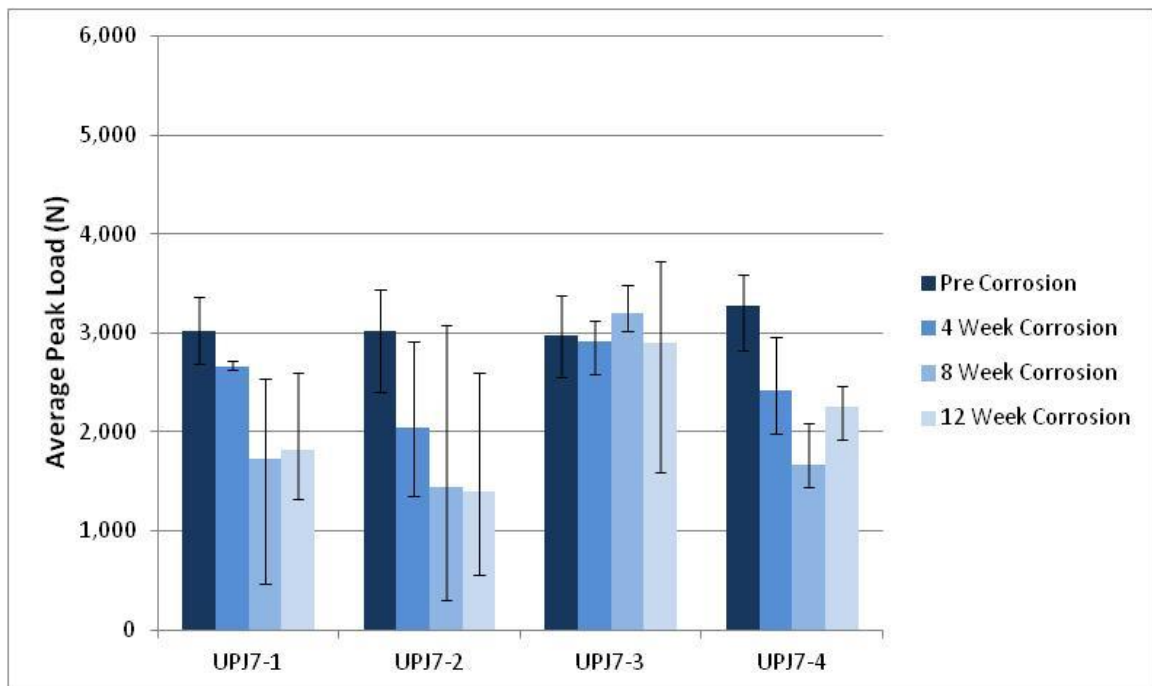


Figure 14. 7-mm round boss UPJ quasi-static cross tension performance prior to corrosion testing and at 4-weeks, 8-weeks, and 12-weeks accelerated corrosion exposure

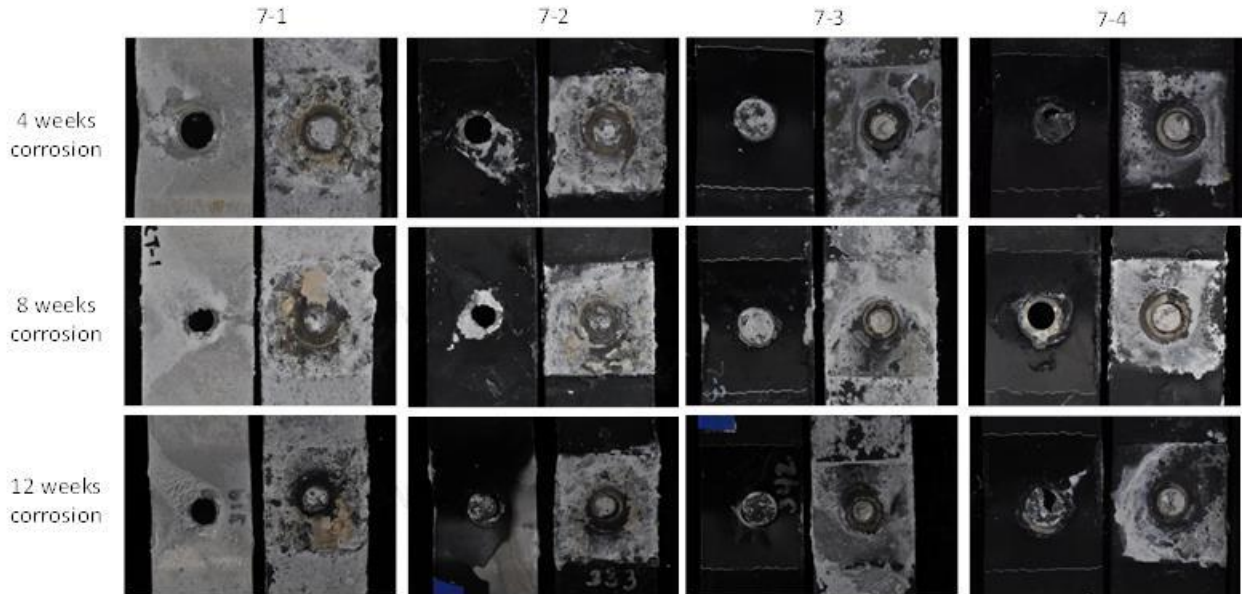


Figure 15. 7-mm round boss UPJ quasi-static cross tension performance failure modes after accelerated corrosion exposure

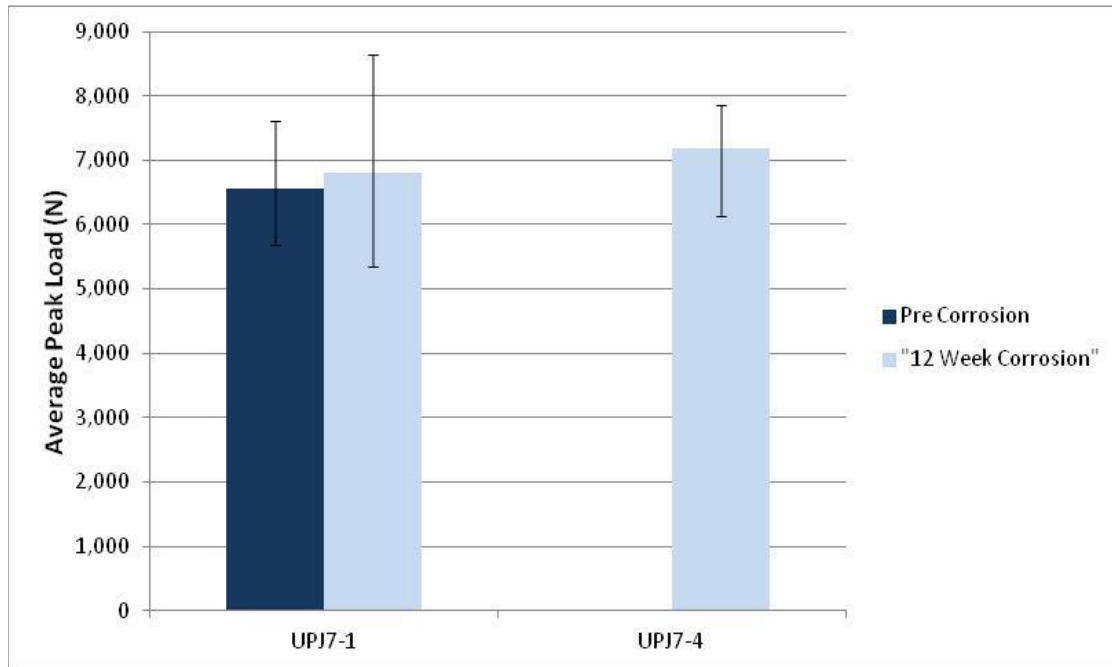


Figure 16. 7-mm round boss UPJ impact lap-shear tension samples prior to corrosion and at 12-weeks exposure

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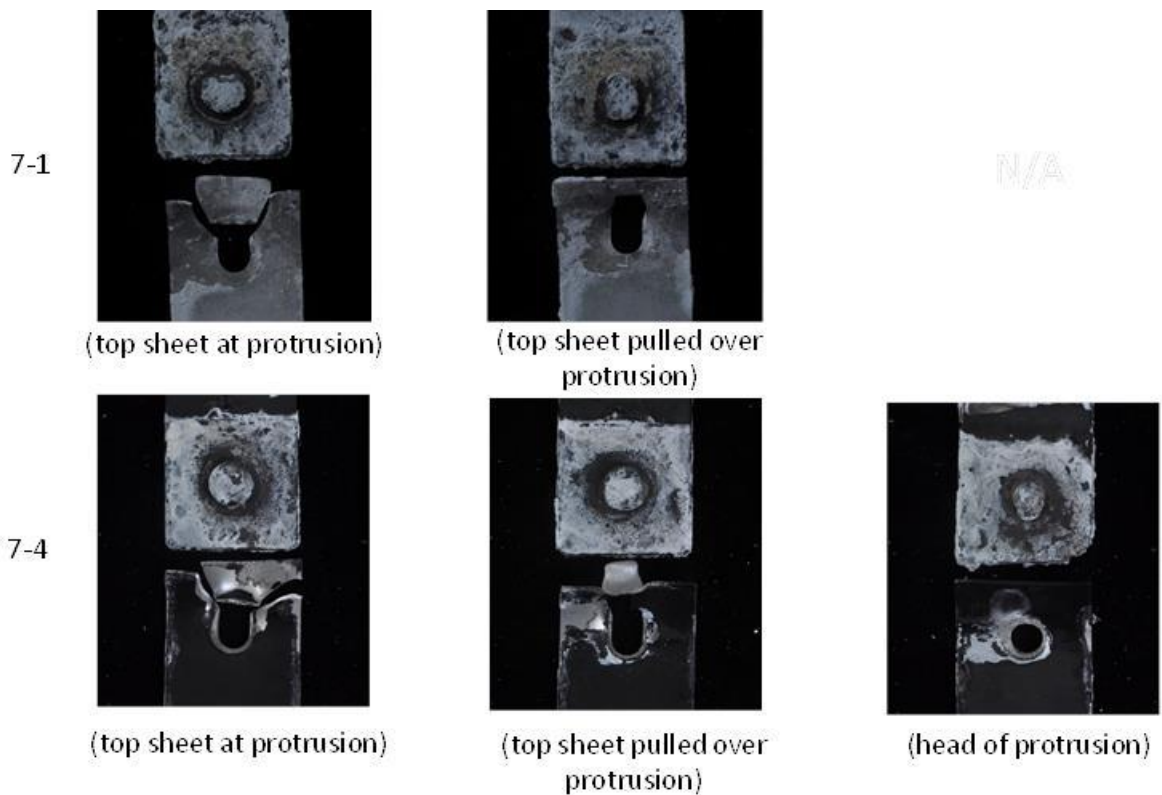


Figure 17. 7-mm round boss UPJ impact lap-shear tension performance failure modes after 12-wks of accelerated corrosion exposure

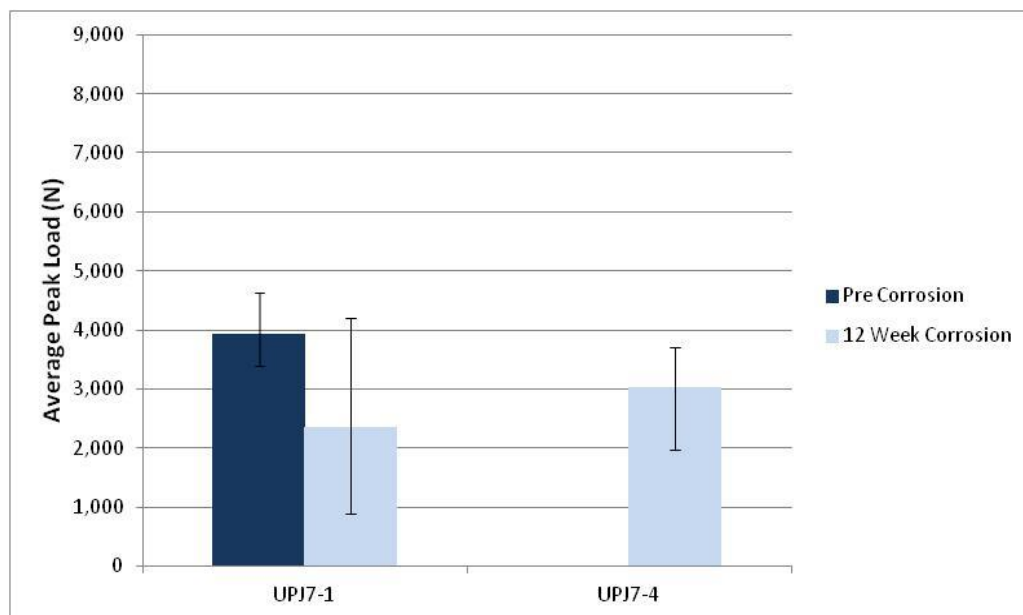


Figure 18. Comparison of round boss UPJ cross tension impact performance prior to corrosion testing and at 12-weeks exposure

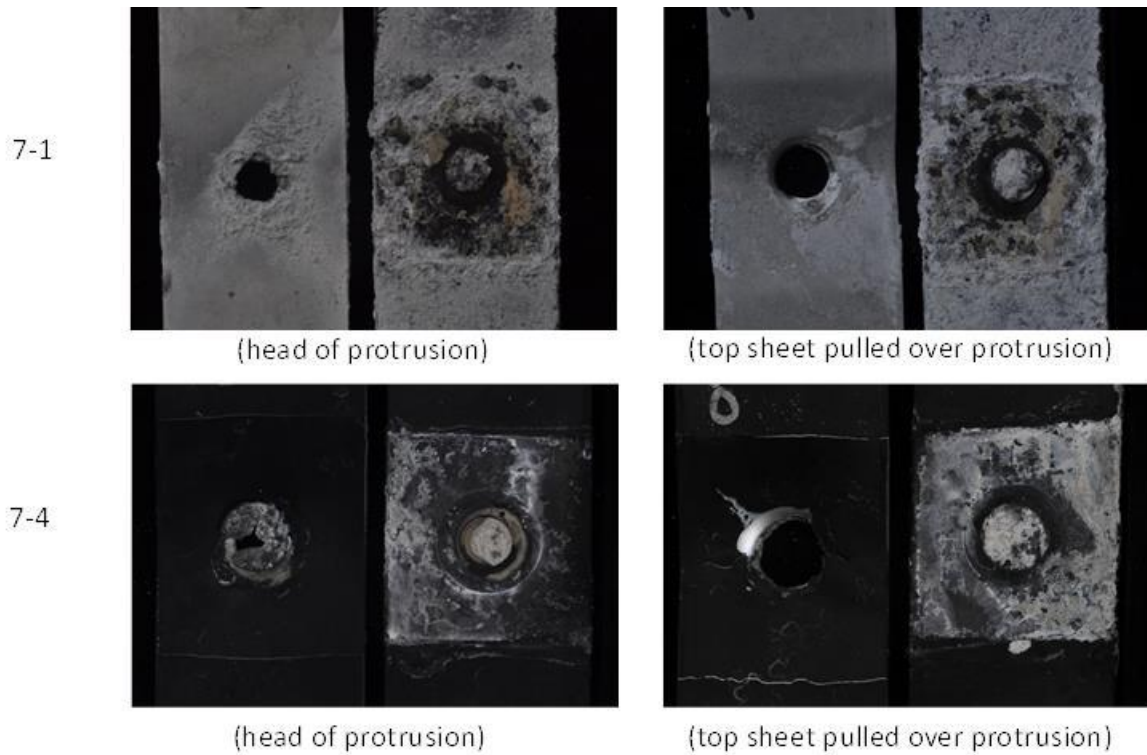


Figure 19. 7-mm round boss UPJ impact cross tension performance failure modes after 12-weeks of accelerated corrosion exposure

Configuration Number	Upper Sheet			Bottom Sheet			Assembly Coating Configuration
	Material	Thickness (mm)	Coating	Material	Thickness (mm)	Coating	
UCR-1	DP590	1.0	Bare	Al 6016-T4	1.3	Bare	Uncoated
UCR-2	DP590	1.0	Armorgalv	Al 6016-T4	1.3	Bare	Uncoated
UCR-3	DP590	1.0	Armorgalv	Al 6016-T4	1.3	Pretreated	Uncoated
UCR-4	DP590	1.0	Armorgalv, e-coat, sealed	Al 6016-T4	1.3	Pretreated	Coated
UCR-5	DP590	1.4	Bare	Al 6016-T4	1.3	Bare	Uncoated
UCR-6	DP590	1.4	Armorgalv	Al 6016-T4	1.3	Bare	Uncoated
UCR-7	DP590	1.4	Armorgalv	Al 6016-T4	1.3	Pretreated	Uncoated
UCR-8	DP590	1.4	Armorgalv, e-coat, sealed	Al 6016-T4	1.3	Pretreated	Coated

Table 2. Round boss UCR material and coating configurations

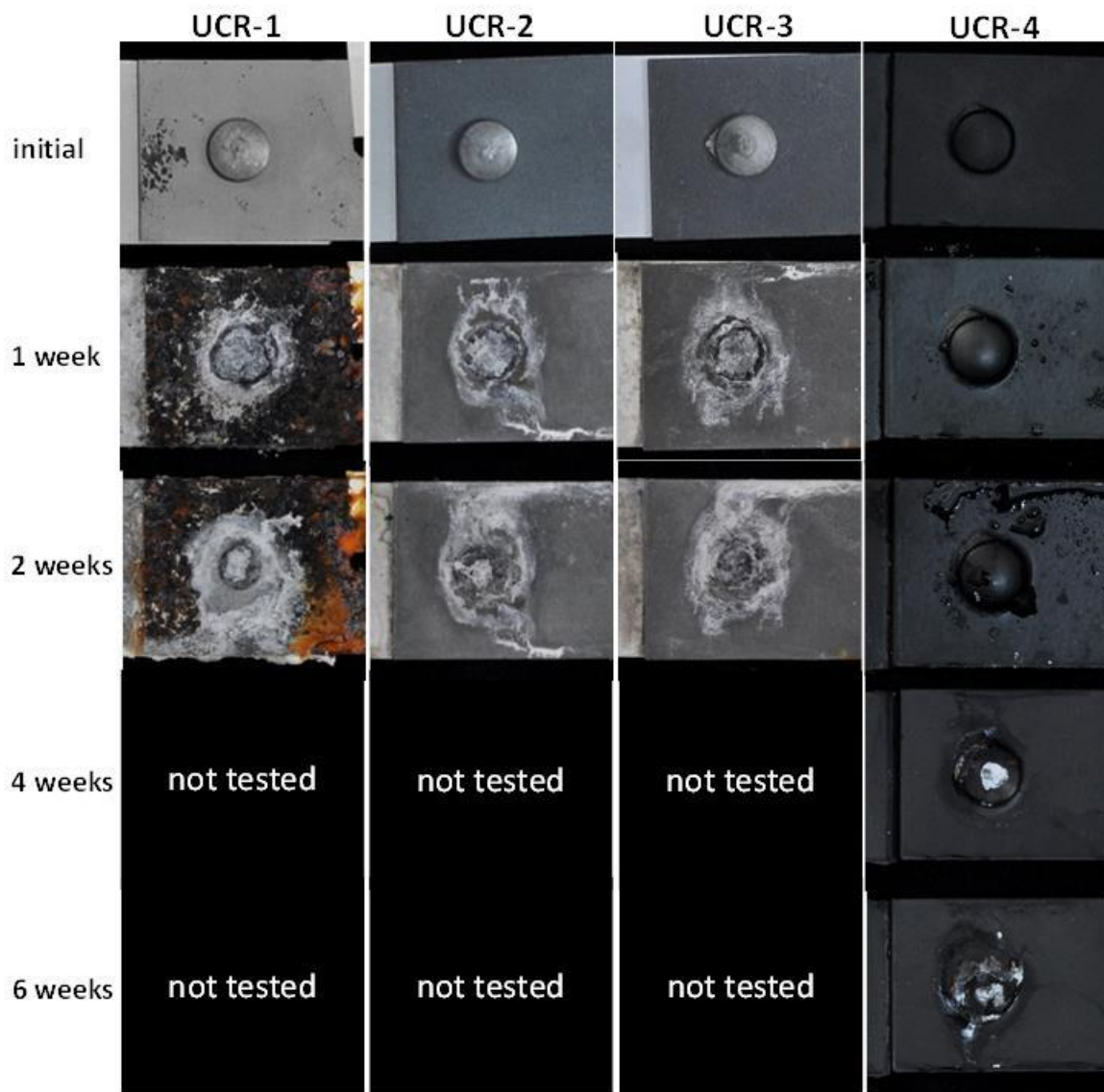


Figure 20. Photos of UCR lap shear joint configurations before and after ASTM G85-A2 accelerated corrosion exposure

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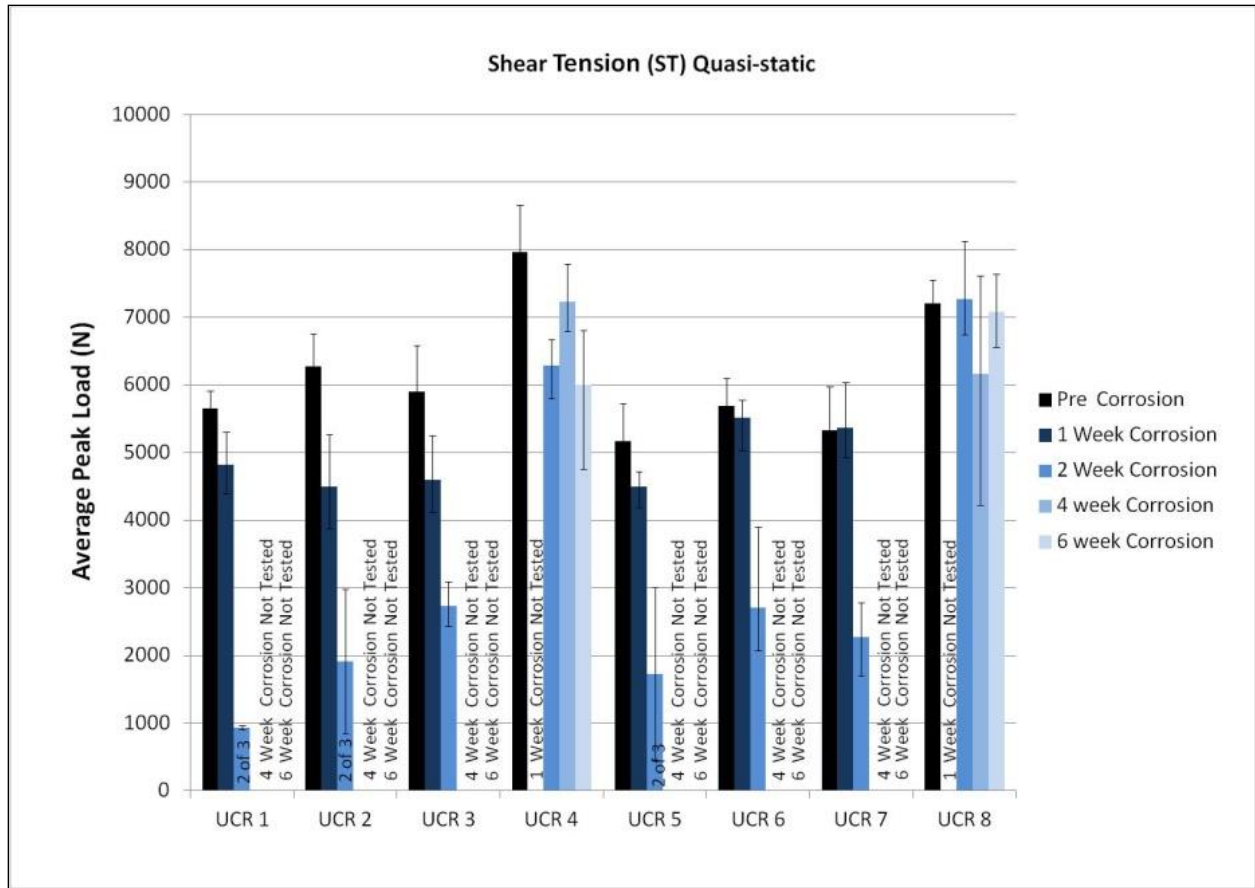


Figure 21. UCR quasi-static lap-shear tension (ST) test results prior to corrosion testing and at 1-week, 2-weeks, 4-weeks, and 6-weeks of accelerated corrosion exposure

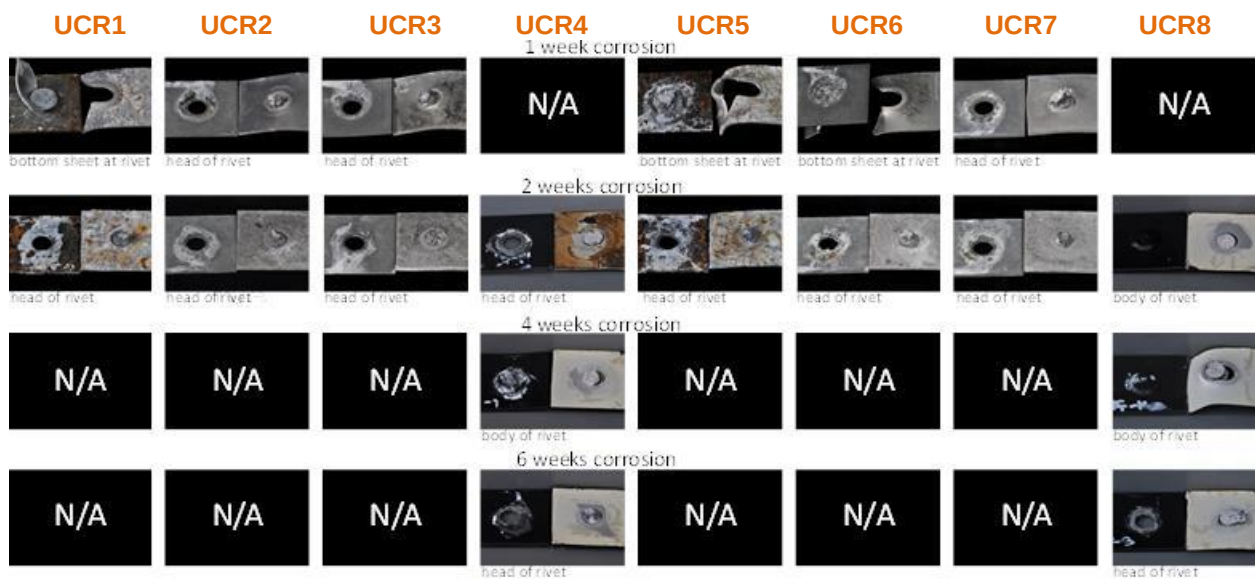


Figure 22. UCR quasi-static lap-shear tension (ST) test assembly failure modes prior to corrosion testing and at 1-week, 2-weeks, 4-weeks, and 6-weeks of accelerated corrosion exposure

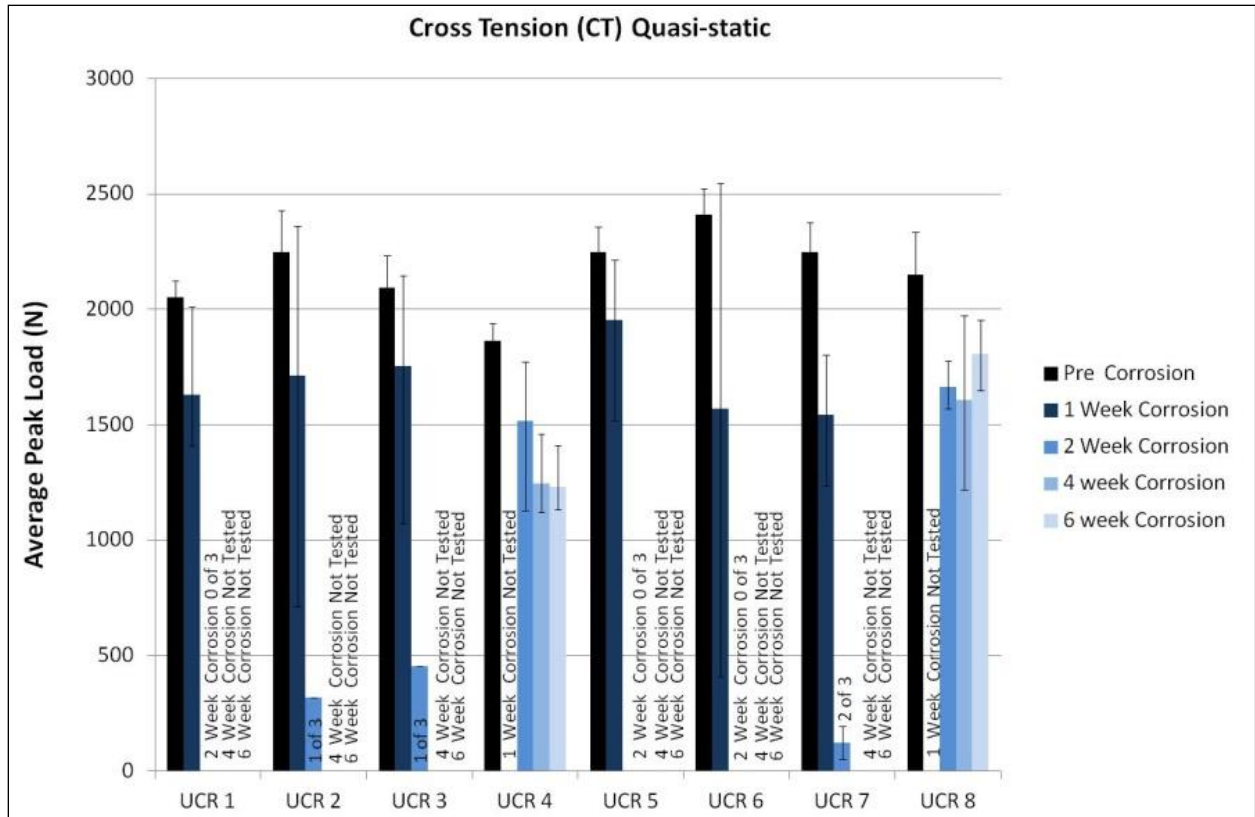


Figure 23. UCR quasi-static cross tension (CT) test results prior to corrosion testing and at 1-week, 2-weeks, 4-weeks, and 6-weeks of accelerated corrosion exposure

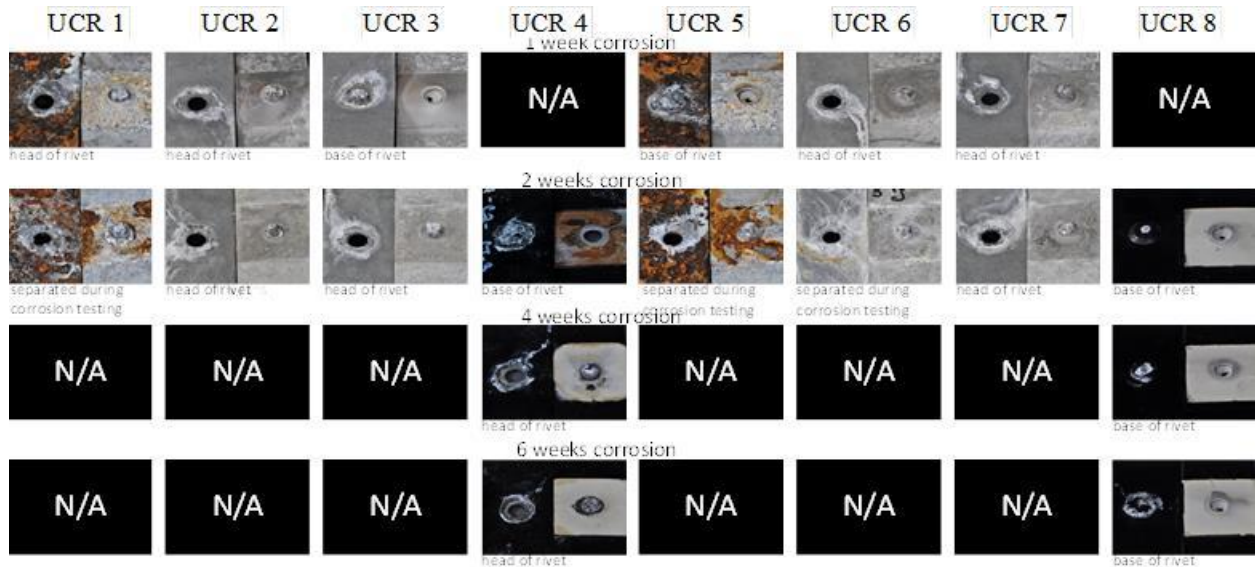


Figure 24. UCR quasi-static cross tension (CT) test assembly failure modes prior to corrosion testing and at 1-week, 2-weeks, 4-weeks, and 6-weeks of accelerated corrosion exposure

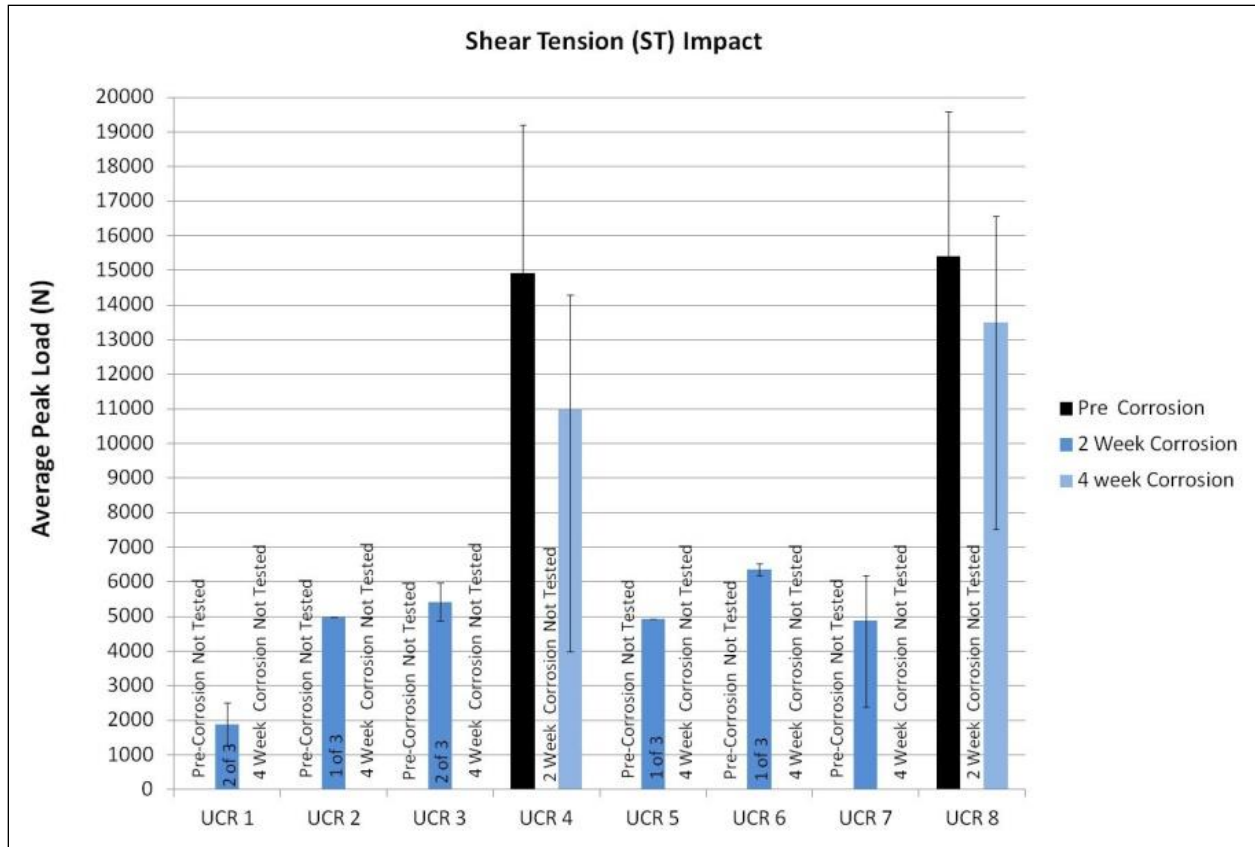


Figure 25. UCR impact lap-shear tension (ST) test results prior to corrosion testing and at 1-week, 2-weeks, 4-weeks, and 6-weeks of accelerated corrosion exposure

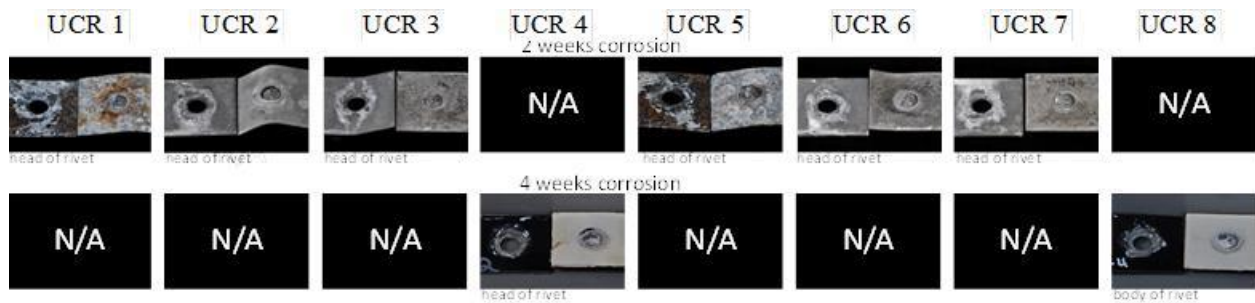


Figure 26. UCR impact lap shear tension (ST) test assembly failure modes prior to corrosion testing and at 2-weeks, and 4-weeks of accelerated corrosion exposure

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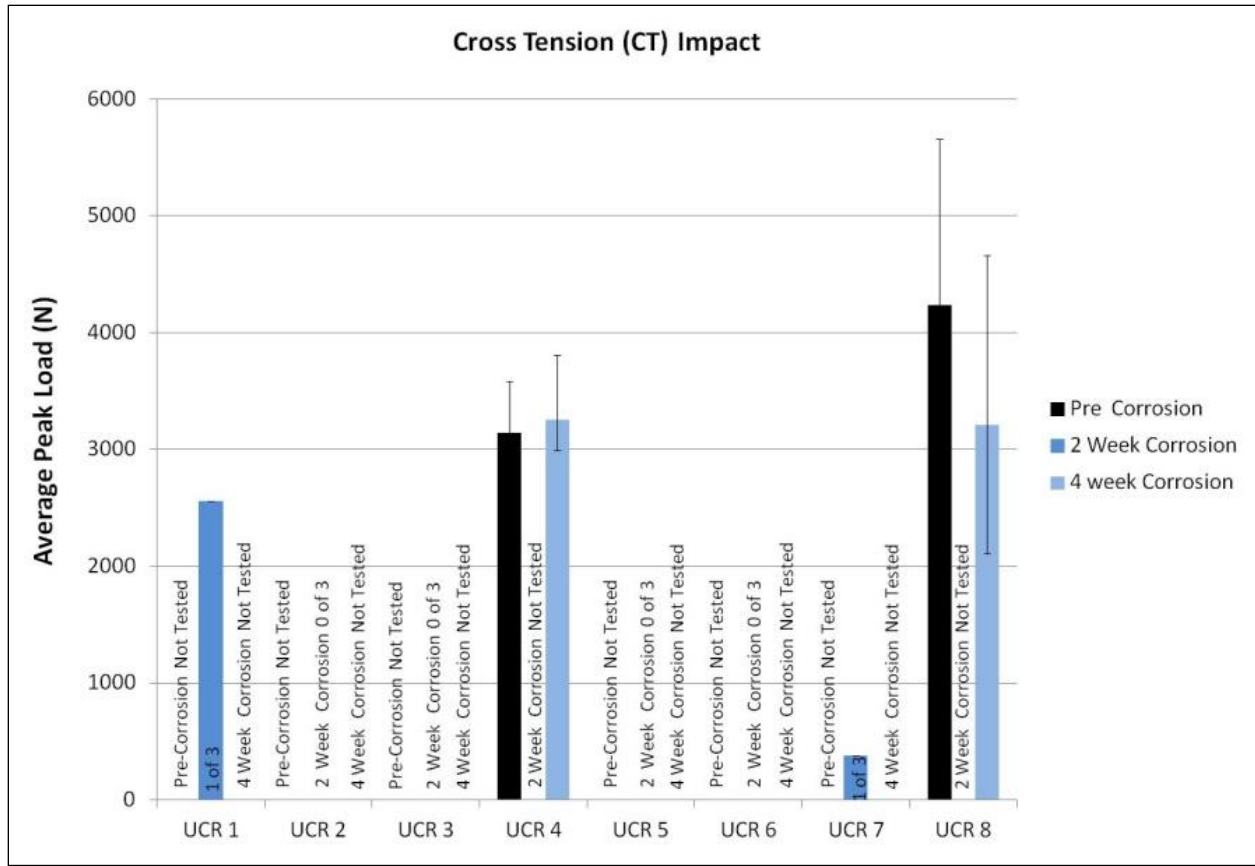


Figure 27. UCR impact cross tension (CT) test results prior to corrosion testing and at 1-week, 2-weeks, 4-weeks, and 6-weeks of accelerated corrosion exposure

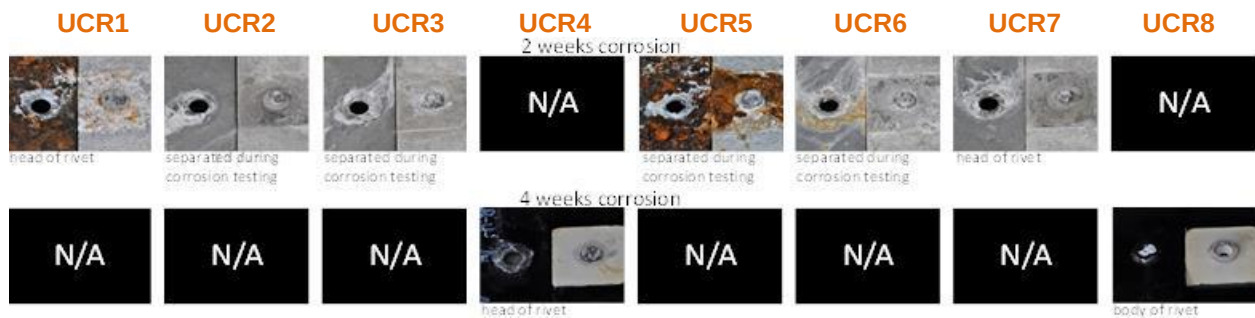


Figure 28. UCR impact cross tension (CT) test assembly failure modes prior to corrosion testing and at 2-weeks, and 4-weeks of accelerated corrosion exposure

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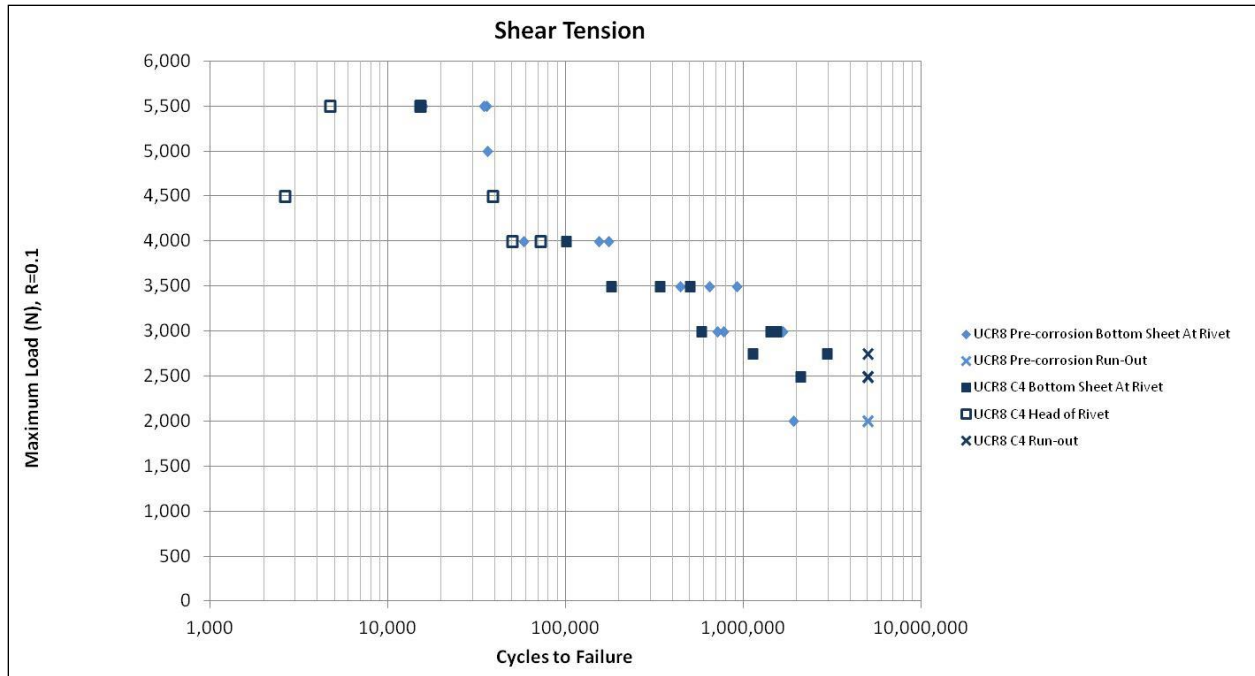


Figure 29. Comparison of UCR8 lap-shear tension fatigue test results prior to corrosion exposure and at 4-weeks exposure

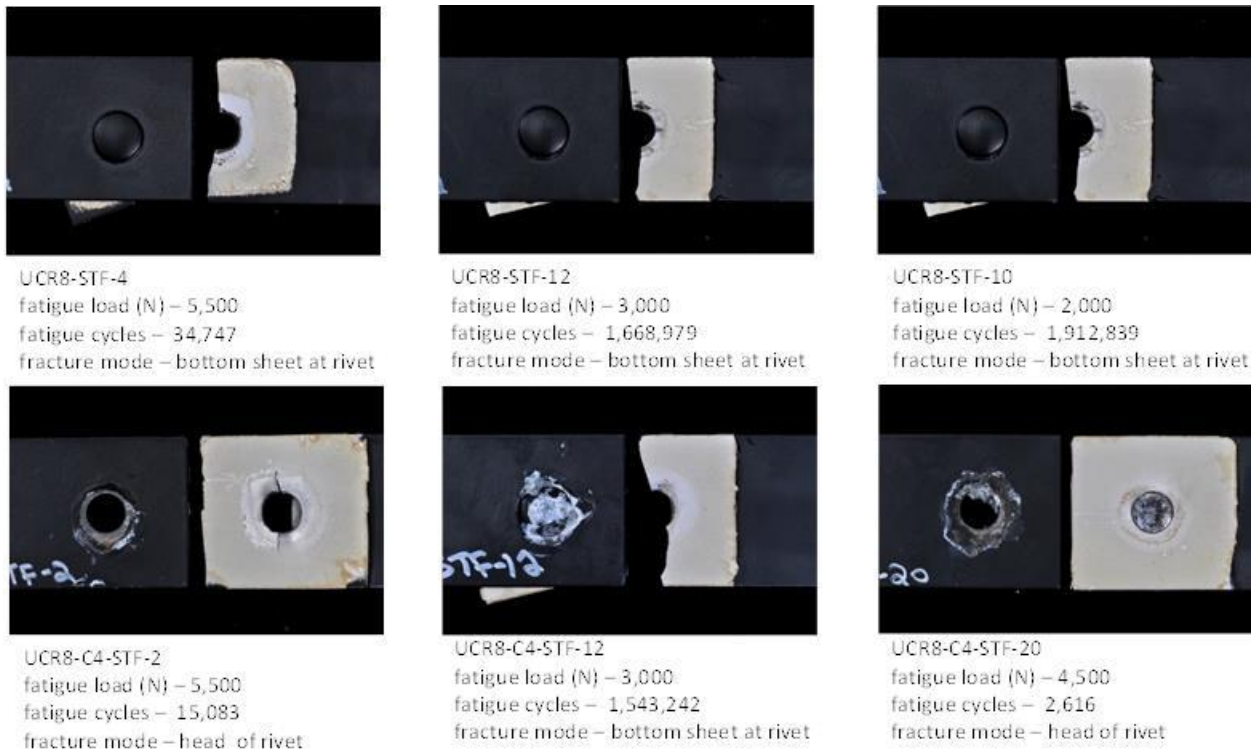


Figure 30. UCR fatigue lap shear tension (ST) test assembly failure mode at 4-weeks of accelerated corrosion exposure (typical failure in bottom sheet parent material)

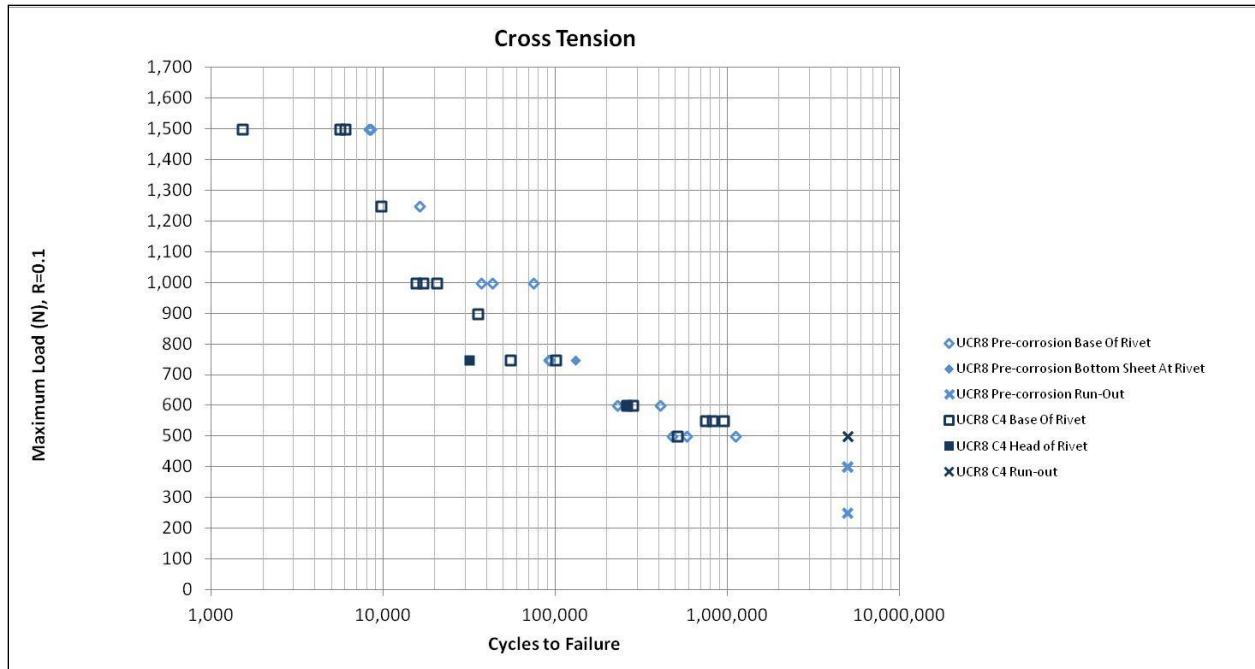


Figure 31. Comparison of UCR8 cross-tension fatigue test results prior to corrosion exposure and at 4-weeks of exposure



Figure 32. UCR fatigue cross tension (CT) test assembly failure mode prior to corrosion exposure (top) and after 4-weeks of accelerated corrosion exposure (bottom). Typical failure is at base of rivet.



Figure 33. Photo of two joined lap-shear tension assemblies utilizing the CARC coating on the steel coupons



Figure 34. Photos of MGC-2.0 treated Mg lap-shear tension coupons (a) prior to contact by the electrode, (b) after application of initial contact force by the electrode but prior to application of electrical current, and (c) after full forming operation with force and current

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AVPTA Technology Focus Area 2: Lightweight Structures & Materials

Breakthrough Techniques for Dissimilar Material Joining – Active, Tailorable Adhesives for Dissimilar Material Bonding, Repair and Reassembly

DOE-VTO TFA Lead: Sarah Ollila
TARDEC TFA Lead: Martin McDonnell

Principal Investigator:
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Project Work was Completed in Q4FY16

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AVPTA Technology Focus Area 2: Lightweight Structures & Materials

Breakthrough Techniques for Dissimilar Material Joining – Laser-Assisted Joining Process for Aluminum and Carbon Fiber Composites

DOE-VTO TFA Lead: Ms. Sarah Ollila
TARDEC TFA Lead: Mr. Martin McDonnell

Principal Investigators:
Dr. Adrian S. Sabau and David C. Warren

Oak Ridge National Laboratory (ORNL)
1 Bethel Valley Road; Oak Ridge, TN 37831

Project Work was Completed in Q3FY16

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AVPTA Technology Focus Area 3: Energy Recovery & Thermal Management

DOE-VTO TFA Lead: Steven Boyd
TARDEC TFA Lead: Mary Goryca

There was no project activity under this TFA during FY16.

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AVPTA Technology Focus Area 4: Alternative Fuels & Lubricants

**Lubricant Formulations to Enhance Fuel Efficiency
Polyalkylene Glycol (PAG) based Lubricant for Light & Medium Duty Axles**

**DOE-VTO TFA Lead: Kevin Stork
TARDEC TFA Lead: Dr. Jay Dusenbury**

**Principal Investigators:
Dr. Arup Gangopadhyay and
Chintin Ved**

Affiliation:
Ford Motor Company
Research and Innovation Center
2101 Village Road
Dearborn, MI 48121

Project Start: Q2FY13
Estimated Completion: Q4FY17

Objectives:

- Develop novel lubricant formulations that are expected to improve the fuel efficiency of medium-duty, commercial and military vehicles by at least 2%
- Develop engine, transmission and axle lubricant formulations, modeling and simulation

Strategic Context:

- This project aligns with TARDEC's LoE 1.4 and Army S&T Challenges to improve operational energy, as well as, DOE's mission to develop more energy-efficient and environmentally friendly technologies.

Accomplishments:

- Developed several candidate polyalkylene glycol (PAG) based axle lubricants. The lubricants have low viscosity and generally improved friction and wear results compared to fully formulated 75W-140 baseline oil.
- Seal compatibility and an industry standardized axle lubricant wear test (i.e., ASTM D6121) was completed on a PAG candidate. Some rebalancing of the additive package required to eliminate rippling issue.
- Dow developed a new oil soluble PAG (OSP) with improved extreme pressure properties and passing rust and copper corrosion, and industry standard test for low speed, high

torque axle operation (i.e., ASTM D6121, L-37), and thermal/oxidation stability (i.e., ASTM D5704, L-60-1).

Introduction:

The objective of this project is to develop novel lubricant formulations that are expected to improve the fuel efficiency of light, medium, heavy-duty, and military vehicles by at least 2% over Society of Automotive Engineers (SAE) 75W-140 axle lubricants (improvement based on comparative results from engine dynamometer testing, chassis dynamometer testing or test track, e.g., SAE J1321) without adverse impacts on vehicle performance or durability.

Approach:

The project objective will be met by completing the following: 1) Lubricant Formulation: Initiate work with the formulation of new polyalkylene glycol (PAG) based axle lubricants. Preliminary testing shall be conducted in an effort to identify those formulations with the greatest potential to meet project objectives. 2) Bench Testing: Evaluate fundamental properties of the new lubricant formulations, test to measure intrinsic properties, physical tests to determine performance characteristics in sliding and rolling friction and wear, micro-pitting, and analysis of lubricant additive-derived anti-wear films using surface sensitive analytical tools. In addition, oxidation and corrosion evaluations will be performed. 3) System and Vehicle Evaluation: Determine performance characteristics in system level (axle) test rigs to evaluate axle efficiency improvements and gear/bearing durability performance of lubricants. Vehicle fuel economy, and potential impact on emissions, will then be demonstrated on a chassis roll dynamometer.

Results and Discussion:

Ford in collaboration with DOW Chemical Company have successfully developed several candidate PAG based axle lubricants. Bench friction and wear testing has been completed at Argonne National Laboratory (ANL) and resulted in improved friction behavior, although ball-on-disc wear results have shown that most PAG candidates did not prevent wear as well as the fully formulated commercial 75W-140. The PAG candidate that showed equal results to the 75W-140 baseline had unacceptable rust test results. Modified PAG candidates were developed but testing showed these 2nd generation candidates resulted in significantly more wear. DOW developed an oil soluble PAG (OSP) candidate that had much improved wear compared to any of the 2nd generation PAG candidates. In addition, the OSP candidate passed both the rust prevention and copper corrosion test. OSP and PAG Gen II formulations were tested in an industry standard test for low speed high torque conditions (i.e., ASTM D6121, L-37) and passed. In addition, both formulations passed the industry standard test for thermal stability (i.e., ASTM D5704, L-60-1). High speed, shock loading testing (i.e. ASTM D 7452) was completed on two OSP candidates. Significant improvements were noted between the first and second formulations but both failed the test requirements. Subsequent investigation identified excessive foaming as main cause of the failures. Investigations into the cause of the foaming were initiated and formulation changes were made to address the issue. Foaming bench tests were conducted and although foaming was significantly reduced, some undesirable foam states still exist. Future project objectives include continued investigation into how foaming can be reduced. Once a

formulation with acceptable foaming has been identified rust (i.e. ASTM D7033, L-33-1), copper corrosion, and an additional L-42 test will be scheduled.

Conclusions:

Ford Motor Company is developing a polyalkylene glycol (PAG) based axle oil, taking advantage of PAG's natural lubricity, high viscosity index, and excellent oxidation and shear stability. In the coming year Ford will continue to identify, test, and evaluate 2nd generation and OSP candidates with additive pack modifications. They will work to solve foaming issues and prepare a final formulation that will pass all the industry standardized tests as well as Ford's propriety axle tests.

Figures and Tables:

None

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AVPTA Technology Focus Area 4: Alternative Fuels & Lubricants

**Lubricant Formulations to Enhance Fuel Efficiency
A Novel Lubricant Formulation Scheme for 2% Fuel Efficiency Improvement**

DOE-VTO TFA Lead: Kevin Stork
TARDEC TFA Lead: Dr. Jay Dusenbury

Principal Investigator:
Dr. Q. Jane Wang

Affiliation:
Mechanical Engineering, Northwestern University
Tech A219, 2145 Sheridan Road
Evanston, IL 60208

Project Start: Q2FY13
Estimated Completion: Q4FY17

Objective:

- Develop novel lubricant formulations for improving the fuel efficiency of light-, medium-, heavy-duty, and/or military vehicles by at least 2% without adversely impacting vehicle performance or durability.

Strategic Context:

- This project aligns with TARDEC's LoE 1.4 and Army S&T Challenges to improve operational energy, as well as, DOE's mission to develop more energy-efficient and environmentally friendly technologies.

Accomplishments:

- Northwestern University has synthesized three major families of heterocyclic additives for boundary lubrication friction reduction.
- These compounds are sulfur and phosphorus free and have produced significant reductions in friction (20 – 40%) and wear (~95%) compared to base oils and fully formulated 5W-30 oil.
- Northwestern University has also developed a method to functionalize solid-state-lubricant nanoparticles (h-BN and B₂O₃) resulting in stable solutions in PAO. Scuffing resistance of the PAO base oil has been increased by a factor of three with 1wt% h-BN nanoparticle.

- Atom transfer radical polymerization (ATRP) with a metallocene catalysis process was utilized in our VM synthesis. 1-octene was converted into a terminal halogen compound effectively via a secondary bromides-initiated hydroboration-bromination reaction.
- In addition to the previous real-time nanoscratch experiments at microscale, entanglement and alignment of the heterocyclic C18Cyc molecules in their surface adsorptions were revealed by MD simulations and characterized by AFM phase mapping, respectively.
- Both tribological and rheological improvements by the randomly-branched PE VM have been identified, indicating that this molecule is a suitable branch block for finalizing the di-block VM synthesis.
- Lubrication performance of a preliminary FM/VM formulation were evaluated under a wide temperature range; more tribological improvements were confirmed for the new additives.

Introduction:

Significant fuel economy benefits can be realized through optimized lubricant formulations utilizing new additive/base oil combinations to control friction, wear, and traction. Northwestern University is synthesizing new friction modifiers (FM) to reduce boundary and mixed lubrication regime friction to enhance the performance of low viscosity lubricants. Northwestern is developing temporary shear thinning viscosity modifiers, and functionalized nanoparticles which reduce friction and wear in the hydrodynamic and boundary lubrication regime respectively.

Approach:

The objective is to be achieved through: (1) reducing friction due to asperity rubbing in start-up and low-speed operations during which boundary friction controls energy dissipation, (2) temporarily reducing the lubricant viscosity (temporary shear-thinning) in medium- to high-speed cruise operations during which viscous loss is the dominant mechanism for energy dissipation, and (3) suppressing oil aeration or foaming responsible for lubrication breakdown in high-speed operations. The proposed research is expected to result not only in at least 2% fuel efficiency improvement, but also enhanced performance of the powertrain/drivetrain components.

Results and Discussion:

More simulation have been done using the MD simulations of the cyclen FMs but with longer side hydrocarbon chains (i.e. C18Cyc). Two models were built before to represent two stages of the adsorption processes for C12Cyc and C12amine molecules, between which the comparison was made and analyzed. This time, for the similar modeling systems built for the C18Cyc and C18amine molecules, MD simulations were also conducted to investigate their surface adsorptions, at both of the beginning stage and the final stage. At the initial stage, the FM molecules were randomly distributed in the space just above the hydrated surface (random model), and they approached the surface from all possible directions. An aligned model was designed for the later stage aiming at capturing the well adsorbed FM molecules in favorable orientations. Figures 1a and 1b show the differences in interaction energies. Temperature effects were considered in the simulations to study desorption and show that the interaction

energies of both FMs under alignment decrease at elevated temperatures, but a desorption process appears for the amine FM molecules only. Fewer and fewer C18amine molecules simulated stay on the surface at higher temperatures, and only about one half of them remain being adsorbed at 200 °C. Meanwhile, the average mass center of the C18Cyc molecules rose by less than 5% due to expanded bond lengths upon heating, but no desorption was found for them at the high temperatures. These results suggest that the C18Cyc FM molecules can be well adsorbed on the surfaces, and this explains a root reason for the greatly enhanced high-temperature boundary lubrication performance found for the heterocyclic FMs.

Polymerization yields have increased greatly since a new Pd catalyst was introduced to the synthesis. The partially synthesized VM possesses a randomly distributed branched polymer block only. An effective thermo-thickening behavior was demonstrated by using less randomly branched PE in the PAO4 base oil. Viscosity index (VI) of the base oil increased by 140 % with the addition of 8 wt% randomly branched PE. An improved shearing performance by this branched polymer block was also found in previous rheological studies. A widely-used commercial OCP (Olefin Copolymer)-based VM was tested for the comparison with the randomly branched PE VM using a pin-on-disk configured tribometer. PAO4 oils with or without 8 wt% of different VMs comprised the lubricants used in this study. Averaged friction coefficients were obtained from the original data, and the standard deviations were used in calculating corresponding errors (see figure 2). The tribological tests started from hydrodynamic lubrication at room temperature and finished at mixed lubrication or boundary lubrications at high temperatures. In general, compared to the commercial OCP VM, the newly synthesized PE VM reduced friction at both speeds tested. The PE VM reduces friction by approximately 20% compared to the commercial OCP VM before entering mixed or boundary lubrication. These tribological and rheological improvements demonstrate the newly synthesized PE VM to be a suitable branchlike polymer block for finalizing the di-block VM synthesis.

A preliminary lubricant formulation was prepared by mixing 1 % of candidate FM (C18Cyc) with the PAO4 oil that contained 8 wt % of the randomly branched PE VM. High-speed pin-on-disk tests were conducted with this preliminary lubricant formulation. Results are shown in figure 3. C18Cyc FM improved the PE VM mixture at high temperatures in boundary or mixed lubrication. A fully formulated synthetic 5W-30 engine oil was also tested and results are shown as blue solid-diamond-dotted curves in Figures 3a and 3b. The lubricant additives and the formulation developed at this current stage of research have exhibited improvements over this commercially available motor oil.

Conclusions:

Northwestern University continues to make progress towards its stated goals. In the coming year they will finalize synthesis of the copolymer viscosity modifier, complete the development of a friction modifier package using the heterocyclic and nanoparticles additives, and develop a strategy for using heterocyclic additives, functionalized nanoparticles, and copolymer viscosity modifiers in a final lubricant formulation.

Figures Begin on Next Page

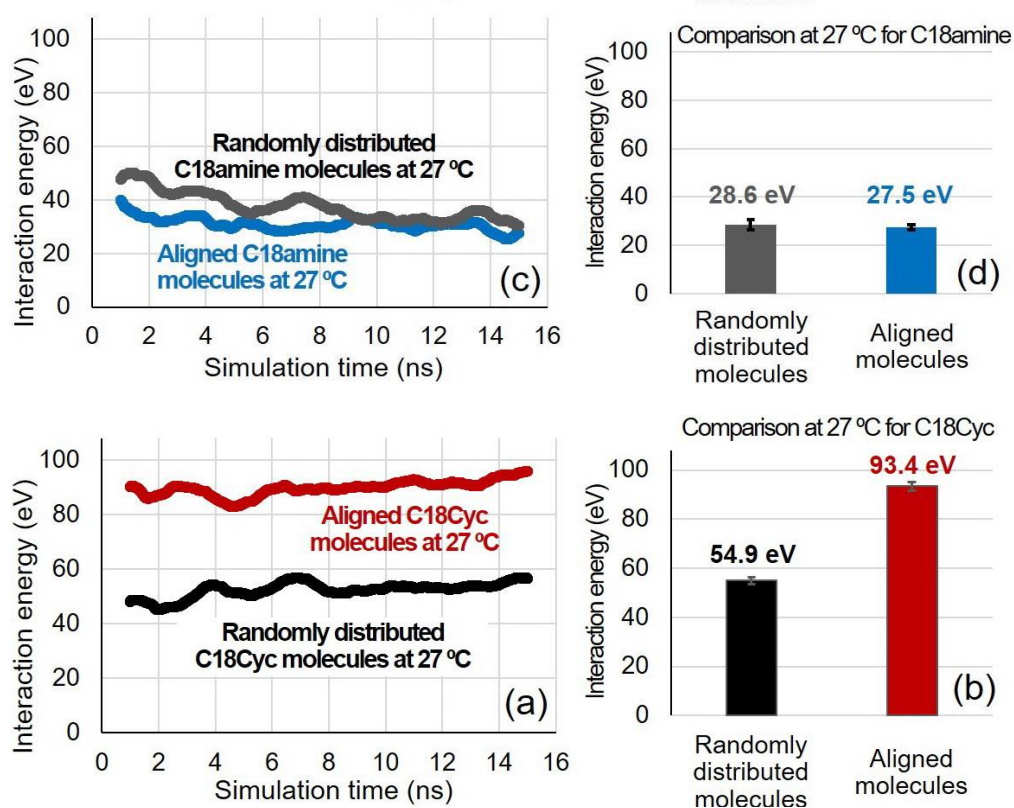
Figures:

Figure 1. Interaction energy of C18Cyc molecules (a) and C18amine molecules (a) versus simulation time; averaged interaction energy (b) of the C18Cyc molecules (b) and C18amine molecules (d) at the last ns.

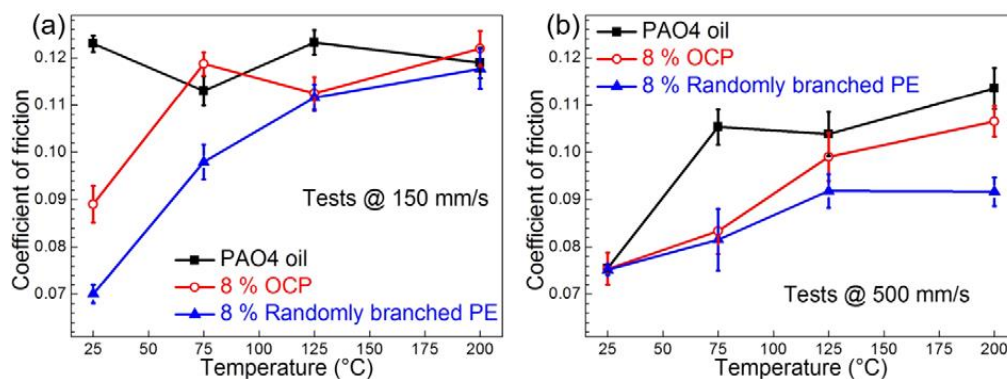


Figure 2. High temperature lubrication test at 150 mm/s (a) and 500 mm/s (b) in PAO4 with or without different VMs.

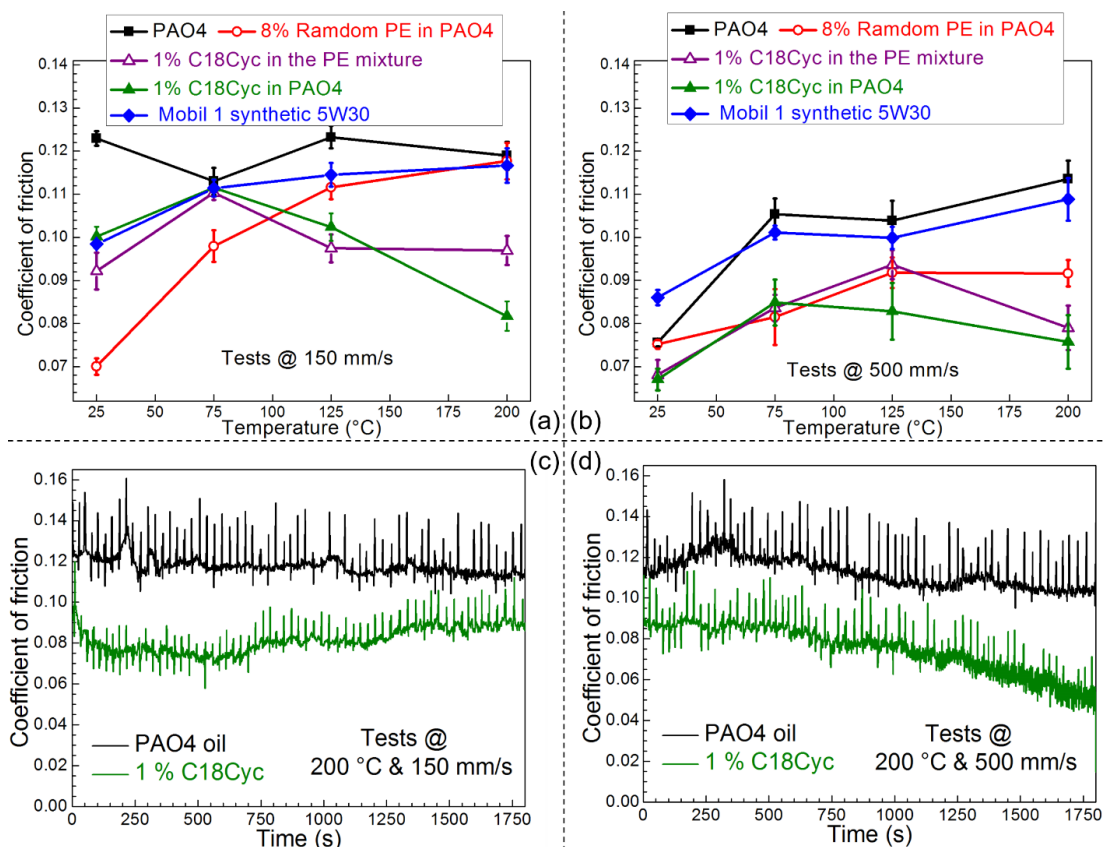


Figure 3. High temperature tests at 150 mm/s (a) and 500 mm/s (b). Friction reduction examples of C18Cyc in PAO4 at 150 mm/s (c) and 500 mm/s (d).

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AVPTA Technology Focus Area 4: Alternative Fuels & Lubricants

**Lubricant Formulations to Enhance Fuel Efficiency
Improved Fuel Economy through Formulation Design and Modeling**

DOE-VTO TFA Lead: Kevin Stork
TARDEC TFA Lead: Dr. Jay Dusenbury

Principal Investigator:
Dr. Gefei Wu

Affiliation:
Valvoline, a Division of Ashland Inc.
3499 Blazer Parkway
Lexington, KY 40509-1850

Project Start: Q2FY13
Estimated Completion: Q4FY17

Objectives:

- Develop novel lubricant formulations that are expected to improve the fuel efficiency of medium-duty, commercial and military vehicles by at least 2%.
- Develop engine, transmission and axle lubricant formulations, modeling and simulation.

Strategic Context:

- This project aligns with TARDEC's LoE 1.4 and Army S&T Challenges to improve operational energy, as well as, DOE's mission to develop more energy-efficient and environmentally friendly technologies.

Accomplishments:

- Valvoline completed transmission testing of baseline and candidate fluid in an SAE#2 test apparatus. Although the low viscosity candidate did not meet the maximum torque and delta torque requirements, they were able to identify a candidate that performed better than the baseline fluid.
- Reformulated two engine oil candidates with PC-11 (FA-4) additive package and found better tribological performance in MTM test while the HFRR and 4-ball test results were mixed.
- Retested two reformulated engine oil candidates at NREL. Both reformulations resulted in better fuel efficiency especially in FTP cycles simulating urban driving cycles.
- J1321 testing is under contract and will begin in November 2016.

Introduction:

The objective of this project is to develop novel lubricant formulations that are expected to improve the fuel efficiency of medium -duty, commercial and military vehicles by at least 2% (improvement based on comparative results from engine dynamometer testing, chassis dynamometer testing or test track, e.g., SAE J1321) without adverse impacts on vehicle performance or durability. This will be accomplished through engine, transmission and axle lubricant formulation design, modeling and testing.

Approach:

Start with fundamental understanding of tribology, lubricant rheology, and oil formulations. Candidate formulations are optimized in the lab using bench tests and analysis led design (mathematical models). Candidate oils are then subjected to engine and/or mechanical testing. Oils with proven lab performance are taken to the field for final validation.

Results and Discussion:

Valvoline has been using their significant experience in lubricant formulation to develop optimized heavy duty diesel engine oil, transmission fluid, and axle oil formulations. Using a baseline CJ-4 15W-40 engine oil, fuel economy testing was conducted at National Renewable Energy Laboratory (NREL) using a Cummins ILS 8.9L engine in two different duty cycles. Engine oil candidate 1 was a 5W-30 oil with HTHS of approximately 3.0. Fuel economy results showed a 1.6% improvement in the FTP cycle and a 1.3% improvement in the SET cycle. Engine oil candidate 2 was a 5W-20 oil with HTHS of approximately 2.8 and used a bio-base oil and friction modifier. Compared with the candidate 1 engine oil, this oil had a higher VI, lower friction and lower traction in bench testing. NREL ISL 8.9L fuel economy testing showed fuel economy improvements 1.8% in the FPT cycle and 1.4% in the SET cycle. For the axle, the baseline is a SAE J2360 approved 75W-90 with proven fuel economy benefits. Axle oil candidate 1 was also a SAE J2360 approved 75W-90. The chemistry had been proven in field testing. Axle oil candidate 2 was a SAE J2360 approved 75W-90 which included Valvoline's proprietary technology. Compared with the candidate 1 axle oil, this oil had a higher VI, higher thermal conductivity and lower churning loss in bench testing. Axle rig efficiency testing showed that both candidates performed better than the baseline in all test conditions and temperature reduction was up to 16.4°C. Efficiency improvement were from 0.63 to 1.36% under demanding conditions. The baseline transmission fluid Valvoline selected was a market leading TES-295 approved fluid. The candidate transmission fluid was to meet the TES-295 performance requirements, but have better efficiency performance. Valvoline conducted nine SAE#2 friction tests. One candidate formula was able to meet the performance target of equivalent or higher maximum torque but lower delta torque. No efficiency evaluations were conducted on this formulation.

Conclusions:

Valvoline has successfully demonstrated significant fuel economy improvements in laboratory bench and dynamometer testing. In the next year of the project Valvoline will conduct SAE J1321 testing to verify an overall fuel economy increase of greater than 2%, conduct final engine durability testing, and investigate the fuel economy retention of its candidate products.

AVPTA Technology Focus Area 4: Alternative Fuels & Lubricants

Lubricant Formulations to Enhance Fuel Efficiency Modified Thermoresponsive Hyperbranched Polymers for Improved Viscosity and Enhanced Lubricity of Engine Oils

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TARDEC TFA Lead: Dr. Jay Dusenbury

Principal Investigator:
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Project Start: Q2FY13
Estimated Completion: Q3FY16

Objective:

- Develop novel lubricant formulations for improving the fuel efficiency of light-, medium-, heavy-duty, and/or military vehicles by at least 2% without adversely impacting vehicle performance or durability.

Strategic Context:

- This project aligns with TARDEC's LoE 1.4 and Army S&T Challenges to improve operational energy, as well as, DOE's mission to develop more energy-efficient and environmentally friendly technologies.

Accomplishments:

- PNNL has completed all of the tasks that involved synthesis and viscosity screening. All synthesized compounds were evaluated by room temperature friction studies at ORNL.
- Three of hyperbranched viscosity modifier (VM) compounds were selected for further friction and wear evaluation at 100°C to provide a means for narrowing down to one candidate for scale-up.
- All blends, base stock with polymer additive, have a lower coefficient of friction (COF) than the base oil. The chosen candidate demonstrated a modest wear increase compared to benchmark additive, which is undesirable, but the COF was lower which should translate into greater fuel efficiency by reducing points of internal friction.

Introduction:

Significant fuel economy benefits can be realized through optimized lubricant formulations utilizing new additive/base oil combinations to control friction, wear, and traction. Any steps taken towards more fuel efficient vehicles will reduce petroleum consumption and by extension and facilitate a cleaner environment. PNNL has focused on designing additives that will lower engine friction and potentially drive train friction, by favorably modifying the lubricant viscosities at high temperatures.

Approach:

Develop and test novel polymers with a hyperbranched architecture as viscosity modifiers and lubricity enhancers to improve fuel efficiency, and ultimately impact fuel economy. The polymers will be engineered to change their molar volume upon heating, thereby increasing the viscosity of the oil, as well as providing terminal groups which will provide the desired lubrication at surface boundaries. The objective for the first component of the project is to design, synthesize and screen molecular structures with hyperbranched architectures for proof-of-concept experiments. This activity includes: 1) designing analogs with the most promising features and easiest to prepare; 2) synthesizing selected compounds; 3) performing screening tests to select the best candidates for further testing. Any design shortcomings will be addressed prior to the second component of the project, which is the tribological and engine testing portion.

Results and Discussion:

PNNL has successfully synthesized several candidate viscosity modifiers (VMs). Friction and wear studies have been completed by Oakridge National Laboratory (ORNL). All candidate VMs resulted in lower coefficient of friction than the base oil, but some also resulted in increased wear compared to a benchmark VM. Based on these results a final candidate VM has been selected for scale up. More than 1000 grams have been produced and will be used for further blend studies and engine testing. PNNL has been working with a major additive supplier to identify an appropriate detergent/inhibitor (DI) package for blending a fully formulated engine oil. A 0W-30 grade engine oil was formulated for final engine fuel economy testing which was conducted by ORNL. The final formulation was tested in a 3-phase Federal Test Procedure (FTP) which included a city fuel economy test, a highway fuel economy test, and a steady-state test. Results were compared against an industry baseline lubricant used in ASTM Sequence VID and VIE and resulted in an improvement of 2.3%, 1.7%, and 1.2% in the city, highway, and steady-state stages respectively.

Conclusions:

PNNL successfully synthesized several candidate viscosity modifiers (VM) and were able to scale up the synthesis process. With help from an industry partner they prepared a 0W-30 engine oil using their proprietary VM technology. The candidate oil was successfully tested at Oakridge National Laboratory where fuel economy testing was completed in accordance with a 3-phase Federal Test Procedure (FTP). Results indicated that PNNL's 0W-30 oil provided improved fuel economy benefits compared to the baseline oil used. Results were greatest under conditions defined as city driving where the improvement was 2.3%.

AVPTA Technology Focus Area 4: Alternative Fuels & Lubricants

Technology Development to Improve Fuel Efficiency through Friction Reduction

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TARDEC TFA Lead: Dr. James Dusenbury

Principal Investigator:
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GW Energy Initiative
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Project Start: Q2FY15
Estimated Completion: Q1FY18

Objectives:

- To develop friction reduction technology capable of improving fuel efficiency of legacy vehicles by at least 2% over the baseline technology using low viscosity lubricants and material technology options (surface textures, diamond-like carbon films, and bonded lubricant films) without sacrificing durability.

Strategic Context:

- Demonstrate a battlefield fuel reduction and reduce the logistics burden.
- Increase Power Density and Energy Efficiency resulting in increased vehicle range, endurance and operational tempo, while reducing the number of logistics convoys on the battlefield.
- Increasing fuel efficiency of ground vehicles to Reduce Life Cycle Costs.

Accomplishments:

- The newly developed 0W-20 “GF-6A” prototype oil was successfully tested in the Seq. VI E tests and the results showed a 2.39% fuel economy over the baseline oil of 2014 GF-5 commercial 0W-30 oil.

- Develop shear, ph and temperature release microencapsulation technology, but have not used in the lubricant that achieved the fuel economy enhancement, further testing must be done to understand and optimize the performance.
- Additives were tested in a 0W-16 formulation where new additive can swap the existing standard ones for evaluation. Most of the new additives yield comparable performance to the standard ones, but are not optimized leaving room for potential performance benefits. Discussions to follow to further pursue and optimize.

Introduction:

In lubricant formulations, base oils of various purities are the solvent and additives are the solute. Additives are added to the solution to impart various performance bench marks. Two types of additives are used, those that control the bulk property such as antioxidants, dispersants, detergents, viscosity modifier (VM), and antifoam; and those that control surface properties, such as anti-wear, friction modifiers, corrosion inhibitors, rust inhibitors, and surface deactivators. The bulk property control agents are either neutrally charged or less polar than the surface active agents; the surface active agents have somewhat hierarchical polarity stacking order to arrange themselves against the sliding surfaces. The anti-wear agent has to be able to adsorb and react with the metal surface to perform its antiwear function, so the decomposition products of the anti-wear agent; ZDDP (zincdialkyl dithio-phosphate) have to react with the surface active sites (3). The formulation has to be delicately balanced to avoid precipitations and adverse additive-additive interactions rendering some or most of the additives non-functioning.

Over the decades, the basic lubricant chemistries have remained the same but modifications to the molecular structures and finer control have been made. The total amount of additives used, however, has grown steadily to accommodate increasing performance demands. Friction modifiers were introduced in the 1980s and a new engine dynamometer test Seq. VI was developed to measure their effectiveness.

Approach:

We propose four tasks to reach the goal (multiple lines of defense against friction deterioration and wear):

Task 1:

Valvoline will supply a commercial SAE 5W-30 GF-5 lubricant to GWU as the baseline formulation. GWU/Valvoline will work jointly to develop a next generation low viscosity fuel efficient lubricant formulation with at least 2% higher fuel efficiency as measured by Seq. VI engine test. GWU will screen new friction reduction chemistry and tougher anti-wear film chemistry in bench tests to identify potential candidates. Valvoline will incorporate the successful candidates into the formulation for testing. The new formulation will be tested to see whether it achieves the fuel efficiency target (as measured by Seq. VI engine tests).

Task 2:

GWU will develop microencapsulation technique (encapsulation, release mechanism, and survivability through engine operation) to create the second line of defense to provide time-release of additives on demand as an option for *Task 1*.

Task 3:

GWU will work with GMC on controlling engine component surface topography and fabricate surface textures to increase film thickness and enable more hydrodynamic lubrication mode in the most significant engine components (identified by GMC) to reduce friction throughout a selected engine model. When the specific engine component operation requires additional durability, GWU will deposit DLC film with bonded chemical film on the engine component to provide robust durability.

Task 4:

The team will integrate the improved engine component (friction surface technology in *Task 3*) with the new energy efficient lubricant to evaluate the combined benefits and robustness of the system durability by bench scale simulation tests for a selected engine component. If the results warrant further testing and development, the industrial partners/and or DOE may consider further investment to commercialize the technology.

Results and Discussion:

Microencapsulation of anti-wear additive poses special challenges compared to encapsulation of other additives. Anti-wear additives such as ZDDP contain strong polar species such as phosphites and phosphates which often interfere with the emulsifiers used in the encapsulation processes. After extensive search and experimentations with various emulsifiers, we finally were able to successfully encapsulate ZDDP, the most common anti-wear additive.

Single additive component multicore capsules have been developed. An attempt was made to encapsulate two to three additives in a single multicore capsule. If this can be achieved, then both friction modifier and anti-wear additive can be injected into sliding contact at the same time. This approach, while desirable, encountered insurmountable barriers. In order to encapsulate sufficient small capsules (<1 micrometer diameter) the shell wall thickness has to be reduced to membranes structure. The small membrane capsules have very large attractive forces among them and they tend to stick together. When we reverted to normal capsule chemistry, the combination of anti-wear additive and friction modifier additive introduced complex interactions rendering them inseparable and cannot be released. We have a single additive multicore capsulation process developed, which meets the milestone shown in Figure 1.

Microcapsules containing single additive component when synthesized, the polymer chemistry and the reaction conditions control the release mechanism of the additive inside the capsules. Literature reported many chemical methods that will preferentially provide triggers to

induce the breaking up of the capsules and release the content. In automobile lubricant applications, most of these methods do not apply since they are related to much weaker structurally capsule polymer chemistry, such as membranes to encapsulate chemicals. The automobile lubricant environment in an operating engine is so severe, that only high melting shear-stable capsules could survive.

After making the capsules to be survivable in engine environment, there are very limited time release mechanisms that can be used. The most useful ones are those release mechanisms based on temperature, shear stress, and acidic of the solution environment. In making capsules, we have adopted a three-step procedure to ensure quality and self-consistency: 1) able to capsule the intended additive; 2) break the capsule manually and recover the additive; 3) compare the recovered additive with virgin additive to ensure the functionality remains the same. In testing the capsules after these three steps, we also would compare virgin additive at a dosage with the capsules added at the same dosage rate that our recovery study revealed. These steps are important to avoid accidental or unrepeatable results.

Since the most important additive in this project is friction modifiers, we chose the friction modifier capsule to illustrate the procedure that we use. Figure 2 shows the results of encapsulated friction modifier tested in a ring and liner tester (Plint TE77) using production ring segment sliding against a production liner segment with cross-hatched surface. The test was conducted at 100°C with reciprocating motion at a speed of 24Hz, step-loading from 30N to 240N with step interval of 6 minutes each.

As can be seen in Figure 2, the oil containing 1.5% friction modifier shows steady friction reduction dramatically from the baseline case. The baseline case friction rises with increased loading approaching a friction coefficient of 0.08 while the oil with 1.5% friction modifier shows after initial steady state friction around 0.036, drops to 0.02 even at the load is increasing. The oil containing the same friction modifier at 1.5% equivalent amount in capsulated form shows an initial COF about 0.04, then rises slightly to 0.042, then continually decrease as the load increases. This is probably due to graduate release of the friction modifier through the temperature and shear trigger mechanisms.

Conclusions:

The project is progressing on schedule. We have successfully fulfilled the major target of the solicitation by meeting 2% fuel economy improvement using the lubricant we have developed, employing various new technologies. Specifically, from test data gathered in the prior annual report, the newly developed 0W-20 “GF-6A” prototype oil was successfully tested in the Seq. VI E tests and the results showed a 2.39% fuel economy over the baseline oil of 2014 GF-5 commercial 0W-30 oil.

We have successfully shown that our capsules have time release properties and now the capsules are ready for trials in real application. The form of trial and how to test their effectiveness are still uncertain since it is a new technology.

The protective coating and chemical films research have been initiated. Meanwhile, the surface texture design and fabrication continues.

Figures:

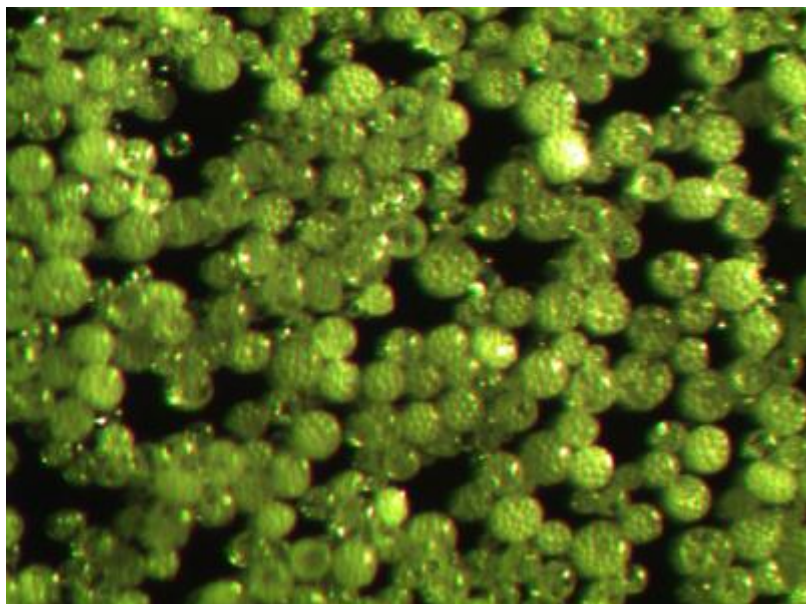


Figure 1. Multicore capsules containing a single anti-wear additive

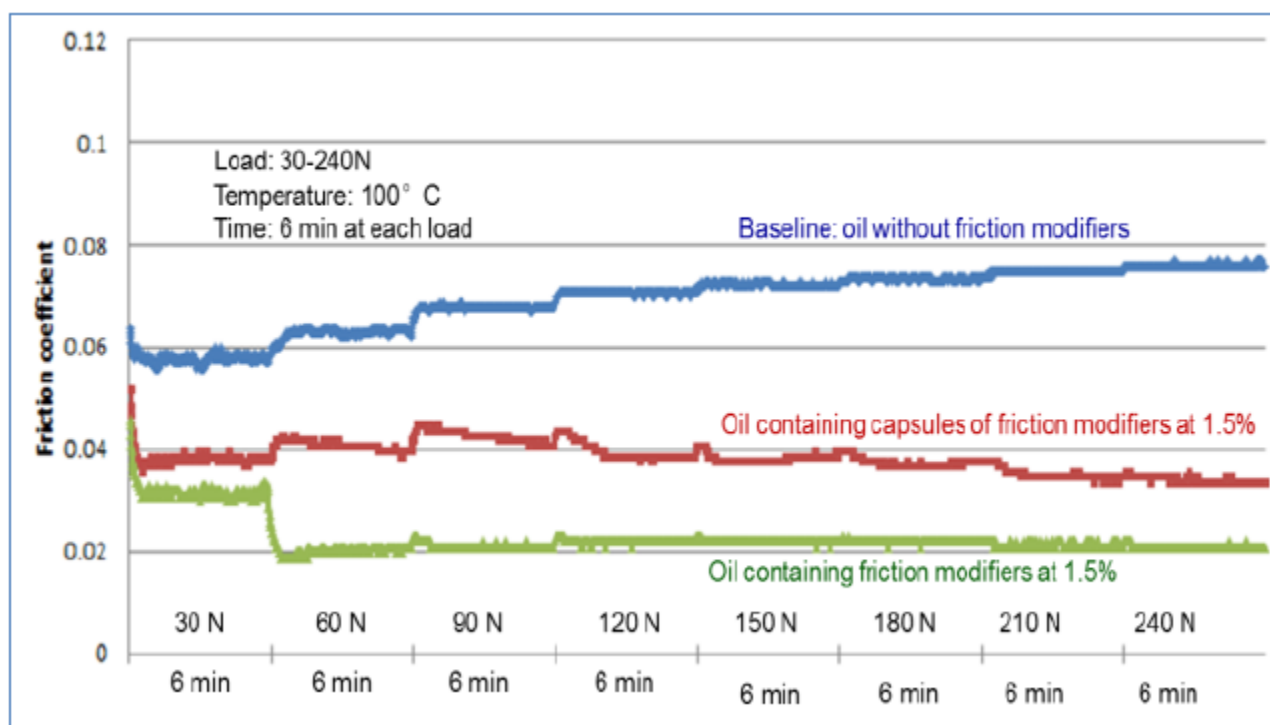


Figure 2. Comparison of encapsulated friction modifier performance among the baseline case that does not contain any friction modifier additive with oil containing 1.5% friction modifier and oil containing 1.5% equivalent friction modifier capsules.

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AVPTA Technology Focus Area 4: Alternative Fuels & Lubricants

Technology Development to Improve Fuel Efficiency through Friction Reduction

DOE-VTO TFA Lead: Mr. Kevin Stork
TARDEC TFA Lead: Dr. James Dusenbury

Principal Investigator:
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Project Start: Q2FY15
Estimated Completion: Q1FY18

Objective:

- To develop and demonstrate friction reduction technologies for light, and medium, vehicles that improve fuel efficiency of future vehicles by at least 4% without adverse impacts on engine durability.

Strategic Context:

- Demonstrate a battlefield fuel reduction and reduce the logistics burden.
- Increase Power Density and Energy Efficiency resulting in increased vehicle range, endurance and operational tempo, while reducing the number of logistics convoys on the battlefield.
- Increasing fuel efficiency of ground vehicles to Reduce Life Cycle Costs.

Accomplishments:

- ANL successfully produced samples of VN-Ni coating on to piston and rings with ~1 μm thickness and no signs of delamination. Further optimization of coating sample piston and rings will continue.
- Liners were received and analyzed for % porosity. The results were encouraging, yielding the desired levels of porosity.
- High Porosity PTWA (HP-PTWA) coatings were achieved.
- Developed a new coating, VN-Ni-Cu, which has been applied to ring segments successfully.

Introduction:

In lubricant formulations, base oils of various purities are the solvent and additives are the solute. Additives are added to the solution to impart various performance bench marks. Two types of additives are used, those that control the bulk property such as antioxidants, dispersants, detergents, viscosity modifier (VM), and antifoam; and those that control surface properties, such as anti-wear, friction modifiers, corrosion inhibitors, rust inhibitors, and surface deactivators. The bulk property control agents are either neutrally charged or less polar than the surface active agents; the surface active agents have somewhat hierarchical polarity stacking order to arrange themselves against the sliding surfaces. The anti-wear agent has to be able to adsorb and react with the metal surface to perform its anti-wear function, so the decomposition products of the anti-wear agent; ZDDP (zincdialkyl dithio-phosphate) have to react with the surface active sites (3). The formulation has to be delicately balanced to avoid precipitations and adverse additive-additive interactions rendering some or most of the additives non-functioning.

Over the decades, the basic lubricant chemistries have remained the same but modifications to the molecular structures and finer control have been made. The total amount of additives used, however, has grown steadily to accommodate increasing performance demands. Friction modifiers were introduced in the 1980s and a new engine dynamometer test Seq. VI was developed to measure their effectiveness.

Approach:

Ford Motor Company (Ford) is investigating a novel way to surface texture engine components in Plasma Transferred Wire Arc (PTWA) coating. PTWA utilizes a cathode tube and plasma gas to sputter low carbon steel from a wire feedstock onto a surface. The scope of this effort includes altering the operating voltage and amperage of this apparatus to control the engine component surface porosity level. Highly porous surfaces could better entrain lubricant and hold it locally even under severe conditions.

Ford is also looking into a nanocomposite coating where a hard metal material (metal oxide or metal nitride) is incorporated into an array of a catalyst material. Argonne National Laboratory (ANL) will be involved for this role due to their expertise and knowledge on development and deposition of nanocomposite coatings on pistons and piston rings.

Results and Discussion:

Nanocomposite coatings have been developed and must be characterized. Scalability and applicability of coatings to piston skirt and piston rings will be determined. Extensive structural, chemical, mechanical and tribological characterization of these coatings using a large variety of microscopic, tribological and surface analytical tools will be completed.

Ford provided ANL with uncoated cast iron liner sections and ring sections. Rings were coated with Nanocomposite VN-Cu coatings. Friction and wear tests were conducted and compared to initial results from HFRR testing. The results showed that the coatings have comparable friction performance compared to the production parts.

All sets of the honed 92.5mm L4 liners were received and analyzed for % porosity. The results were encouraging, yielding the desired levels of porosity and sample cross sections can be found in Figure 1. Porosity measurements quantified that High Porosity PTWA (HP-PTWA) coating were achieved.

Evaluation began for high porosity PTWA coatings began on ring coatings and textured connecting rod bearings using motored component level tests. Currently, the freestanding confirmation liners and bi-material friction liners are being sprayed and machined at four different levels to support various performance tests during BP2. These liners were manufactured, prepped, sprayed and machined and are currently being honed and machined to the final specs. Friction tests were initiated using the TE77 Plint friction test rig to assess the performance of coatings in various lubrication regimes and the wear scars with microscopy imaging can be seen in Figure 2.

Conclusions:

ANL has developed a new coating, VN-Ni-Cu. The new coating has been applied to rings segments successfully.

HP-PTWA was successfully developed and Ford will prepare and provide HP-PTWA coated liner sections to ANL to be tested against the new nanocomposite coated rings.

All of the 2.0L custom made cylinder blocks were machined, prepped and are ready to be sprayed. Two of the blocks will undergo coating deposition and machining trials to establish manufacturing process for friction tests. These blocks will support motored wear testing and cranktrain friction testing in BP3.

Single cylinder test rig was redesigned to allow for pressurization. Modifications to existing rig were completed in 2ndQ 2016.

Discussions are underway with a number of suppliers regarding Ring, Bearing, Piston and Texturing technologies to support the upcoming performance tests.

Figures Begin on Next Page

Figures:

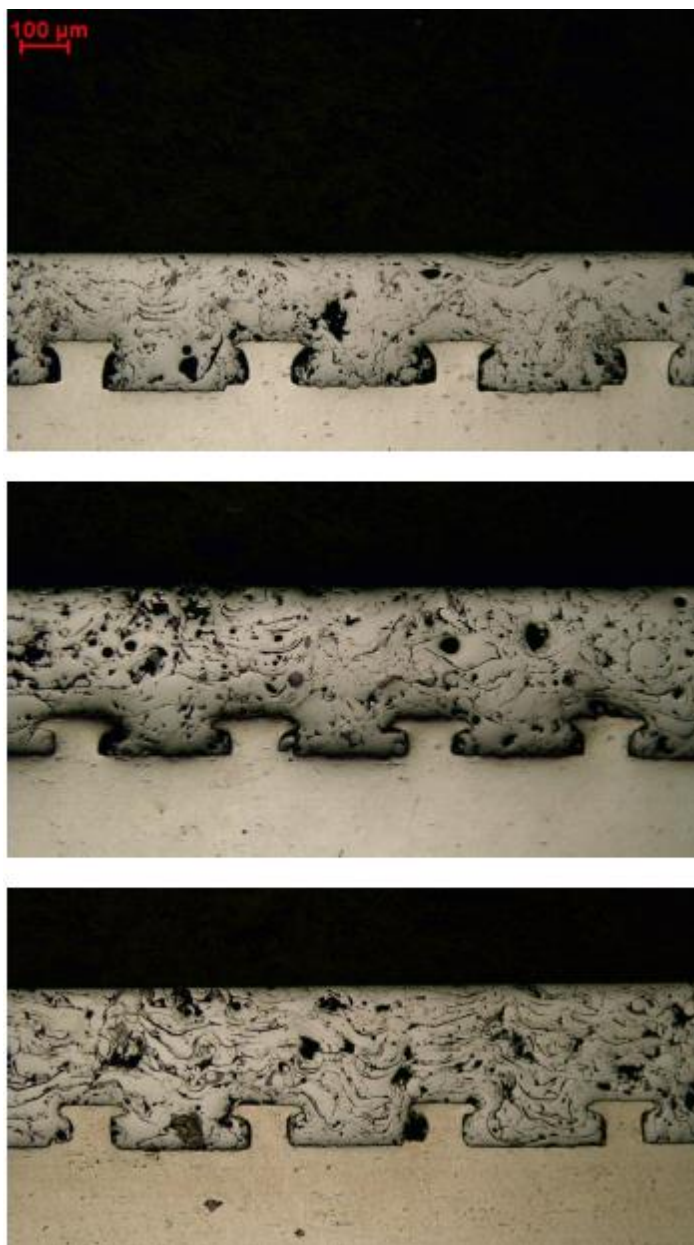


Figure 1. Cross section of multiple process trial liners showing coating's microstructure and porosity.

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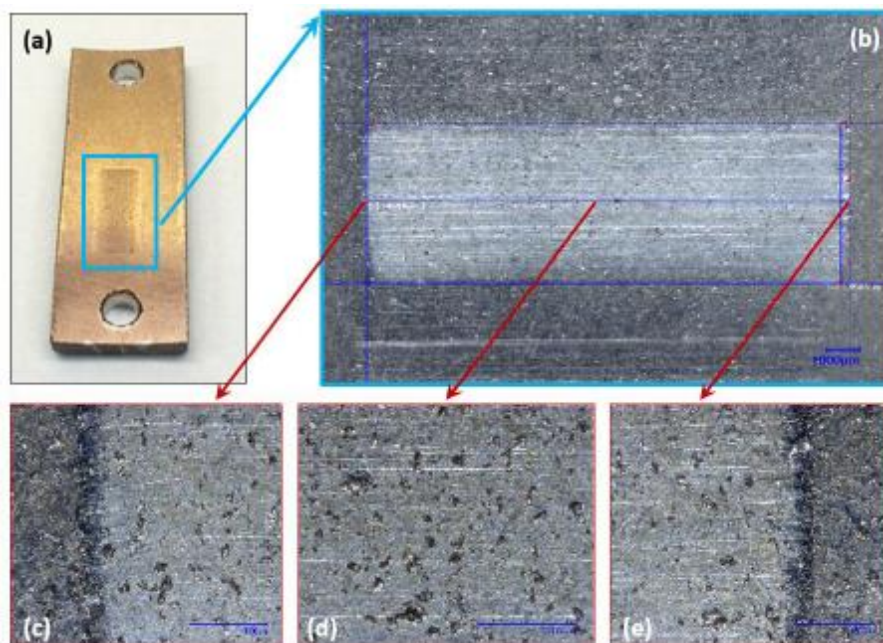


Figure 2. (a) A Plint TE77 test coupon after the friction test showing the contact area; (b) Close-up of the contact area to measure contact length and width; (c), (d) and (e) Micrograph of contact area at different locations used for wear assessment and porosity measurement.

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AVPTA Technology Focus Area 4: Alternative Fuels & Lubricants

Technology Development to Improve Fuel Efficiency through Friction Reduction

DOE-VTO TFA Lead: Mr. Kevin Stork
TARDEC TFA Lead: Dr. James Dusenbury

Principal Investigator:
Dr. Jun Qu

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Project Start: Q4FY15
Estimated Completion: Q3FY18

Objectives:

- To further develop the ionic liquid-additized low viscosity engine oil meeting the GF-5/6 specifications and possessing superior lubricating characteristics.
- Expand the ionic liquid additive technology to rear axle lubricant to gain a combined 4% improvement in vehicle fuel economy.

Strategic Context:

- Demonstrate a battlefield fuel reduction and reduce the logistics burden.
- Increase Power Density and Energy Efficiency resulting in increased vehicle range, endurance and operational tempo, while reducing the number of logistics convoys on the battlefield.
- Increasing fuel efficiency of ground vehicles to Reduce Life Cycle Costs.

Accomplishments:

- Synthesis of copper nanoparticles (NPs) at two different sizes, 24nm and 15nm.
 - Computer simulation of nanoparticles was initiated during this quarter which included
 - Validation of the simulation's ability to correctly predict solubility of polymer functionalized NPs with varying molecular structures
 - Initial development of modelling NPs in boundary lubrication on the atomic scale.
- The optimal ratio between ZDDP and IL has been found. The [1:1] ratio outperformed the rest ratios [1:3, 1:2, 2:1, and 3:1] in wear reduction.

- Synergistic IL+ZDDP combination exhibits promising performance at treat rates as low as 0.1%
- Milestone: Finalization of the multi-grade viscosity of the candidate engine oil: The milestone has been met. SAE 0W-12 has been determined as the main target while SAE 0W-8 is not fully excluded.
- Performed Tribological screening tests on PAO 4 cSt base oil additized by ionic liquid together with two different ZDDPs (anti-wear additive) to investigate the impact of IL+ZDDP on friction.

Introduction:

On 9/28/2013, the ORNL-GM team successfully concluded a 4-year joint project sponsored by DOE Vehicle Technologies Office (VTO) under a Cooperative Research and Development Agreement (CRADA) for developing ionic liquids as next-generation AW additives for engine lubrication. This team made a major breakthrough in developing new groups of oil-miscible ionic liquids (ILs)³⁻⁷, with high thermal stability, ashless, non-corrosiveness, and most importantly effective AW characteristics. Fundamental investigation has correlated the anti-wear and friction reduction mechanisms of IL additives to their physical (absorption) and chemical (tribofilm formation) interactions with the metallic bearing surfaces³⁻⁵. In addition, accelerated catalyst aging tests of the IL suggested potentially less adverse effects on three-way catalysts compared to ZDDP⁶. Working with Lubrizol, the team had developed a prototype IL-additized fully-formulated automotive engine oil (the first ever in the literature). The IL-additized engine oil has low-viscosity (comparable to the pending SAE grade 8) and has demonstrated promising lubricating performance⁶. High-temperature, high-load (HTHL) engine tests showed similar engine wear and oil aging behavior between the IL-additized low-viscosity engine oil and the Mobil 1 5W-30 engine oil⁶. Further, Sequence VID engine efficiency dynamometer tests of this prototype IL-additized engine oil demonstrated an improved fuel economy by 2.01% benchmarked against the Mobil 1 5W-30 engine oil⁶. The initial success of our ionic liquid additive technology has been highlighted at Inside Science⁸ and Green Car Congress⁹, and starts gaining interest from both academia and industry.

Approach:

There are a number of bearing components in an automotive vehicle. The second largest parasitic friction induced energy loss is the 3-5% at the rear axle (next to the 10-12% in the engine)^{1, 2}, and therefore is identified as the next application for the IL additive technology. GM's modeling predicts a potential recovery of 0.75-1.5% vehicle fuel economy by using a lower viscosity oil. This study proposes to apply ionic liquids to mitigate the challenge of wear protection induced by the reduced oil viscosity. The bearing interface for the rear axle is very different from that in the engine, therefore the IL chemistry will be tailored to better handle the much higher contact stress and longer oil service life required for the rear axle lubricant. This study will also provide us the opportunity to gain deeper fundamental understanding of ILs' anti-wear mechanism such as the roles of the cations and anions, and their advantages in surface absorption and tribofilm formation compared to conventional neutral AW additives. Such understanding will strengthen the scientific basis that we have been building for further material optimization and product development.

ORNL will be leading this joint project with main responsibilities for IL design and synthesis, tribological bench tests, tribofilm characterizations, lubrication modeling, and emission analysis. GM will work with Lubrizol to formulate IL-additized engine and rear axle lubricants. GM will conduct complementary tribological bench tests, multi-cylinder engine dynamometer tests, and vehicle tests.

Results and Discussion:

An investigation to find the optimal ratio between ZDDP and IL was performed. The $[P_{888}][DEHP]$ ionic liquid+ZDDP at [1:1] ratio outperformed the rest ratios [1:3, 1:2, 2:1, and 3:1] in wear reduction which satisfied a project milestone.

Our previous work has shown synergistic effects on friction and wear reductions when combining a phosphonium-organophosphate IL and ZDDP [1]. Chemical analysis indicated remarkably 30-70x higher concentrations of the IL and ZDDP active elements than the nominal values on the fluid surface and hypothetical anion-exchange produced new compounds, which may explain the superior tribological performance and distinct tribofilm composition [1]. This suggests a possibility of using a lower treat rate of IL+ZDDP combination to still gain sufficient wear protection.

Tribo-tests were conducted on a series of concentrations, 0.92%, 0.46%, 0.23%, and 0.1%, of IL+ZDDP at [1:1] ratio in a PAO 4 cSt base oil. Ball-on-flat reciprocating sliding tests were performed with an oscillation frequency of 10 Hz and a stroke of 10 mm. AISI 52100 hardened steel balls of 10 mm diameter were used to rub against the cast iron flats for 1000 m under 100 N at 150 °C. The P contents of 0.8% ZDDP and 1.04% IL in PAO both were 800 ppm. The 0.92%, 0.46%, 0.23%, and 0.1% of IL+ZDDP correspond to 800 ppm, 400 ppm, 200 ppm, and 87 ppm of P content, respectively, in the base oil. The wear results are summarized in Figure 1. Using ZDDP or IL alone effectively reduced the wear, but were outperformed by IL+ZDDP at the same 800 ppm phosphorus content. Interestingly, a half treat rate (0.46%) of IL+ZDDP performs as well as the full amount (0.92%). A linear, increasing trend in wear rate was observed for the concentrations of IL+ZDDP decreasing from 0.46% to 0.1%, but the 0.1% IL+ZDDP (87 ppm P) still outperformed the 0.8% ZDDP and 1.04% IL (both 800 ppm P).

Results suggest that the synergistic IL+ZDDP combination may maintain its maximum wear protection at a half concentration and still outperform ZDDP alone even at a concentration one order of magnitude lower. This reduces the phosphorus content from 800 ppm to less than 100 ppm, which would significantly reduce the adverse impact on exhaust emission catalysts.

GM received two ZDDPs (A and B) from Lubrizol and investigated their impact on friction and wear using tribotests on a mini traction machine (MTM2). Stribeck curves were generated first under 75 N at 100 °C with a 50% sliding rolling ratio followed by wear tests for 15 hrs. In both repeat tests, the PAO 4 base oil failed prematurely due to scuffing, after ~20 and ~30 min testing, respectively. ZDDP-A and -B additized PAO oils were able to finish the 15 hrs tests in all 3 repeats. The stribeck curves and wear volumes (disc + ball) of PAO, PAO+0.8%ZDDP-A, and PAO+0.8% DDP-B are compared in Figure 2. As expected, the addition of ZDDPs

eliminated the scuffing failure with much lower wear rates but moderately increased the mixed and boundary friction. These results set the baseline for further tests on PAO + IL and PAO + (IL+ZDDP).

SAE 0W-12 has been determined as the main target while SAE 0W-8 is not fully excluded which met a milestone.

GM performed tribotests on PAO 4 cSt base oil additized by [P₈₈₈][DEHP] (IL) together with two different ZDDPs provided by Lubrizol to investigate the impact of IL+ZDDP on friction by using a mini traction machine (MTM). ZDDP-A is a secondary ZDDP with 10 wt% phosphorus content, and ZDDP-B is a primary ZDDP with 7 wt% phosphorus content. In Figure 3, stribek curves were generated under 75 N at 100 °C with a 50% sliding rolling ratio. For IL + ZDDP, IL was added at 0.52% for 400 ppm P, and ZDDP was added at either 400 ppm P (0.4% ZDDP-A or 0.57% ZDDP-B) or 800 ppm P (0.8% ZDDP-A or 1.14% ZDDP-B). The addition of an IL+ZDDP combination increased the mixed and boundary friction less than using a ZDDP alone. We plan to use a multiple Stribeck scans, an approach described in [1], in the coming quarters to further understand the impact of the growth of IL+ZDDP tribofilm on friction in all lubrication regimes.

Conclusions:

The optimal ratio to demonstrate the synergy between ZDDP and IL was found to be 1:1 based on an experimental tribological investigation. The target low viscosity fuel efficient oil was found to be SAE 0W-12, which will be pursued. The synergistic effect between ZDDP and IL should allow superior surface protection under boundary lubrication, thus, moving to a lower viscosity lubricant could be feasible.

Anti-wear additive concentration was investigated using the optimal ratio between ZDDP and IL using a benchtop tribometer. There is now an understanding of how much concentration is necessary to provide adequate surface protection avoiding excess wear, scuffing and seizure.

Stribeck mapping was performed on IL and IL-ZDDP fluids to investigate the frictional performance of these novel lubricants. Stribeck mapping will be conducted in multiple trials going forward to understand how the performance changes as the steel surfaces change and tribofilms grow.

Figures Begin on Next Page

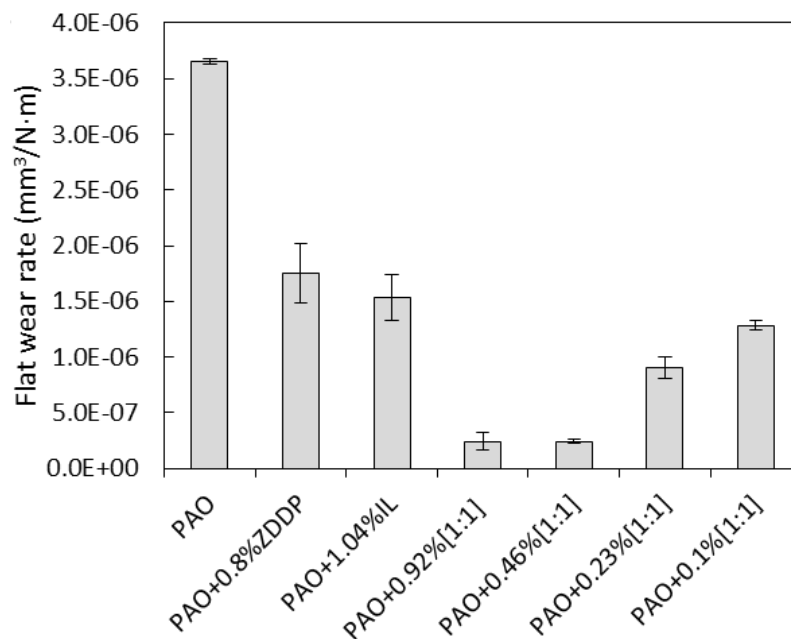
Figures:

Figure 1. Wear rates in PAO 4 base oils containing combined IL+ZDDP at treat rates of 0.92%, 0.46%, 0.23%, and 0.1%. Results show that 0.46% IL+ZDDP (400 ppm P) maintains the maximum wear protection and 0.1% IL+ZDDP (87 ppm P) outperforms 0.8% ZDDP alone (800 ppm P).

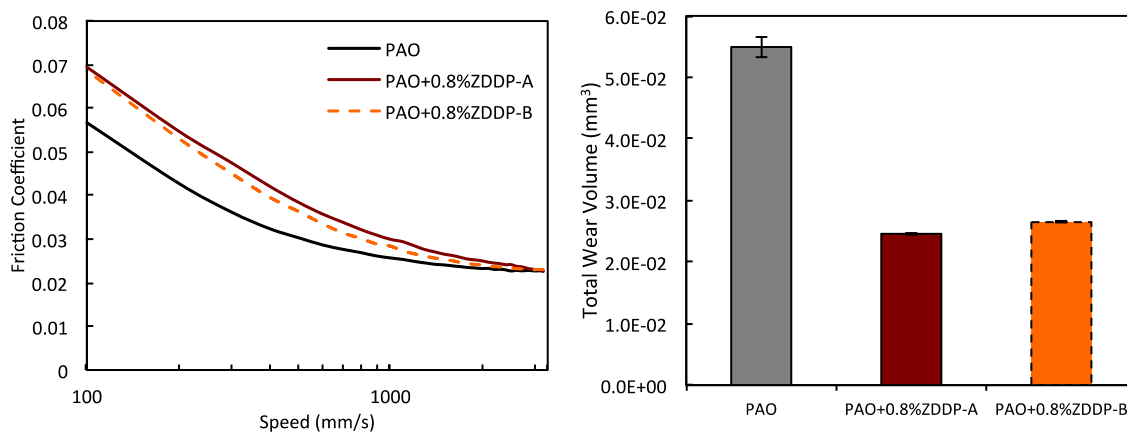


Figure 2. Stribeck curves and total wear volume of PAO, PAO + 0.8% ZDDP-A, and PAO + 0.8% ZDDP-B from a mini traction machine.

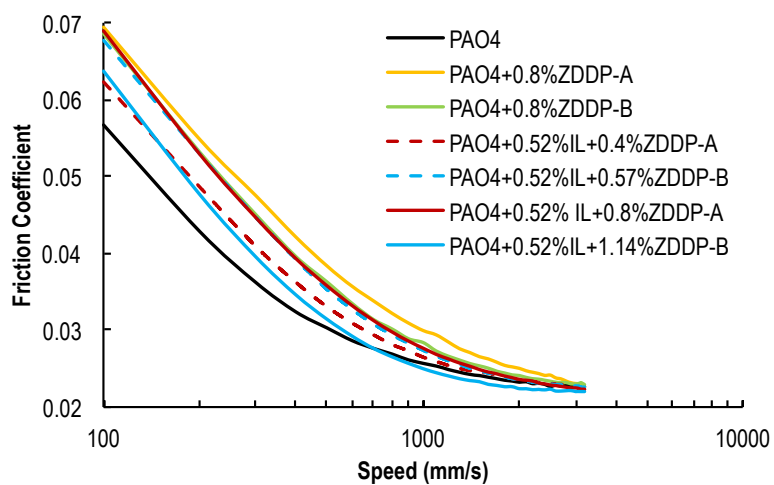


Figure 3. Stribeck curves for PAO4, PAO4 + ZDDP, and PAO4 + IL + ZDDP by using MTM.

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AVPTA Technology Focus Area 4: Alternative Fuels & Lubricants

Technology Development to Improve Fuel Efficiency through Friction Reduction: Method to Measure, Predict and Relate Friction, Wear and Fuel Economy

DOE-VTO TFA Lead: Kevin Stork
TARDEC TFA Lead: Dr. Jay Dusenbury

Principal Investigator:
Dr. Steve Gravante

Affiliation:
Ricardo, Inc.
40000 Ricardo Drive
VanBuren Township, MI 48111

Project Start: Q1FY15
Estimated Completion: Q2FY16

Objectives:

- To provide the lab-scale fundamental data (open source), model correlations, and full scale verifications to enable more accurate predictions of friction coefficient and wear for a wider range of engines, lubricants, and operating conditions than currently exists.
- To extend the approach to sliding and rolling friction in gears.

Strategic Context:

- Demonstrate a battlefield fuel reduction and reduce the logistics burden.
- Increase Power Density and Energy Efficiency resulting in increased vehicle range, endurance and operational tempo, while reducing the number of logistics convoys on the battlefield.
- Increasing fuel efficiency of ground vehicles to Reduce Life Cycle Costs.

Accomplishments:

- A RINGPAK model was developed to simulate the reciprocating motion of lab-scale testing.
- Lab-scale testing of base Isuzu parts (ring-on-liner) has been completed
- RINGPAK model setup for the ANL setup is complete and best practice development and validation has started
- Skirt-on-liner testing at ANL w/ low & high viscosity oil has been completed

- Full-scale testing at EMA of base Isuzu components (ring-on-liner & skirt-on-liner) w/ low & high viscosity oil continues to make progress
- Preliminary sensitivity study of RINGPAK model predictions to key inputs has been conducted. Agreement has been improved between prediction and measured friction coefficient.

Introduction:

Friction forces and wear performance in engines and other driveline components can be calculated from equations that capture the understanding of the fundamental physics involved. However, accuracy of the results is dependent on measurement or estimation of the friction coefficient used in the calculations. For contacting surfaces in any component system (piston ring or skirt and liner; bearings; gears, etc.) the friction coefficient is a function of lubricant viscosity, relative speed, surface properties and load, which is captured in a Stribeck curve.

For a given set of operating conditions the curve provides a friction coefficient which can be used to calculate FMEP (Friction Mean Effective Pressure). FMEP is a quantification of losses due to friction during engine operation. It combines all types of friction losses from asperity or boundary friction (caused by metal to metal contact) to hydrodynamic friction (caused by viscous losses) and mixed regimes between. Once FMEP is quantified, whether predicted or measured, it can be used to calculate friction impacts on fuel economy.

Approach:

In this program Ricardo will use existing computer models to specify relevant Stribeck conditions (speed and load) for light duty and heavy duty OEM engines (one or more of each). ANL and EMA will make careful measurements of friction and wear using high-precision lab-scale test rigs as a function of surface and lubricant properties over a range of operating temperatures, loads, and speeds typical of engine (or other) components. The data generated will be used, with some processing, as input to Ricardo's codes to improve correlations between model FMEP predictions and measurements of FMEP in full scale engine or driveline tests.

FMEP is equal to the difference between IMEP (Indicated Mean Effective Pressure), which is the theoretical amount of power the engine can produce from the amount of fuel burned, and BMEP (Brake Mean Effective Pressure), which is the amount of power delivered by the crankshaft. Because FMEP is the relatively small difference between two relatively large numbers, accuracy can be poor when determining FMEP by calculating IMEP and subtracting measured BMEP. It can be measured directly in motored tests, but they lack some of the physical realities (temperatures, combustion forces, etc.) of fired engines. Methods to calculate FMEP from well verified models are needed.

The "technology" developed in this project will be FMEP maps as a function of load and speed which, when coupled with IMEP, can be used with suitable weighting factors to predict fuel consumption for any user-specified driving cycle. The lab-scale rig data will be used to predict wear loads (cycle averaged as a function of speed and load) to compare with wear-load-sliding distance calculations. Lubricant effects will be evaluated in terms of both friction losses and wear performance. The models will be used to predict fuel savings and wear, as validated with engine dyno tests by Ricardo and Navistar using an off-the-shelf high viscosity lubricant

and a friction-modified low-viscosity synthetic lubricant. Engine tear-down tests at INL will provide data on engine component wear in fleet-tested vehicles.

Results and Discussion:

Effort has continued to validate the reciprocating test Ringpak model developed to simulate the benchtop tests being performed on Isuzu rings and cylinder liner segments. It consists of segments of the top compression ring (from the Isuzu engine) that are reciprocated back and forth against a segment of the cylinder bore. Tests have been performed at a range of loads (50, 250, and 500 N), at different temperatures (70, 100, and 130 °C, and a few at nominal room temperature), and at speeds ranging from 1 Hz up to 5 Hz (20 mm stroke).

A series of tests have been performed to obtain information on the asperity/boundary friction coefficient for use in subsequent RINGPAK and PISDYN simulations of friction in fired Isuzu engine dyno tests.

The runs at 100 °C exhibited nearly 'square-wave' behavior indicating that at 100 °C, the friction is predominantly boundary friction – little or no mixed or hydrodynamic friction (see Figure 1).

At room temperature however, the friction trace was 'scalloped' (see Figure 22), indicating friction was a mixture of boundary and mixed – boundary at the end/reversal points where the speeds were low, and mixed at the mid-stroke where the speed and viscosity were such that partial film formation was occurring.

A version of the Ricardo RINGPAK code was developed to model the benchtop experiments. The model configuration is shown in Figure 22 – it consists of a piston inside of a cylinder bore with a single piston ring. The AART RINGPAK model uses an exceptionally long connecting rod (10 m) coupled with a short crank offset to minimize side forces. The normal force between the ring and the cylinder bore is mimicked by controlling the ring tension. A number of AART RINGPAK simulation runs were performed to model the frictional behavior of the configuration shown in Figure 3 (nominal room temperature, 5 Hz, 50 N). The 50 N normal loading (spread over an assumed track of 10 mm corresponds to a ring tension of approximately 600 N.

The variables that were considered in the simulation study included temperature, oil viscosity, speed, load, film thickness, materials, asperities and surface finish.

After considerable analysis, a set of parameters were established that when used with the AART RINGPAK model would accurately predict the friction forces and traces. The data in Figure 4 shows a comparison of the experimental friction coefficient with the predicted frictional trace assuming the following conditions: 40 °C, 0.1 asperity friction, GWT parameters consistent with an as-received liner (MATUTIL), inlet oil film thickness of 10 µm.

Conclusions:

The results are sensitive to the inlet oil film thickness, especially for values below 1 μm . Values below 1 μm result in significant asperity friction and are unrealistic to the flooded condition used in the experiment. Above 1 μm , the results are not sensitive to this parameter. Ring tension has a significant effect and caution must be taken to use the correct value. Initial analysis assumed the 50 N load was distributed over a contact length of 10 mm. In reality, the contact width is dependent on a number of factors including load and radius of curvatures of the ring and bore coupons. More detailed analysis (Tribology ABC) suggests a contact width of 6-8 mm corresponding to a unit loading of 7 N/mm (900 N Fd) is more appropriate.

Temperature plays an important role. In particular, the role of frictional heating and surface heating needs to be considered. While frictional power at the interface may be low (less than 1 watt), a simple estimate using simple conductive heat flow ($-kAdT/dx = q$) suggests a ΔT of 40 $^{\circ}\text{C}$ is reasonable.

The surface finish plays a significant role in the simulation. The agreement with the experiment in Figure 4 was achieved using GWT parameters (as derived with the MATUTIL package) for an as-received/unworn surface. When GWT parameters for the worn surface were used, the friction trace was dominated by hydrodynamic lubrication – the asperity-to-asperity friction was significantly reduced. We are currently investigating the procedures used by MATUTIL used to calculate the GWT parameters to determine how they compare with other methods to calculate GWT parameters.

Figures:

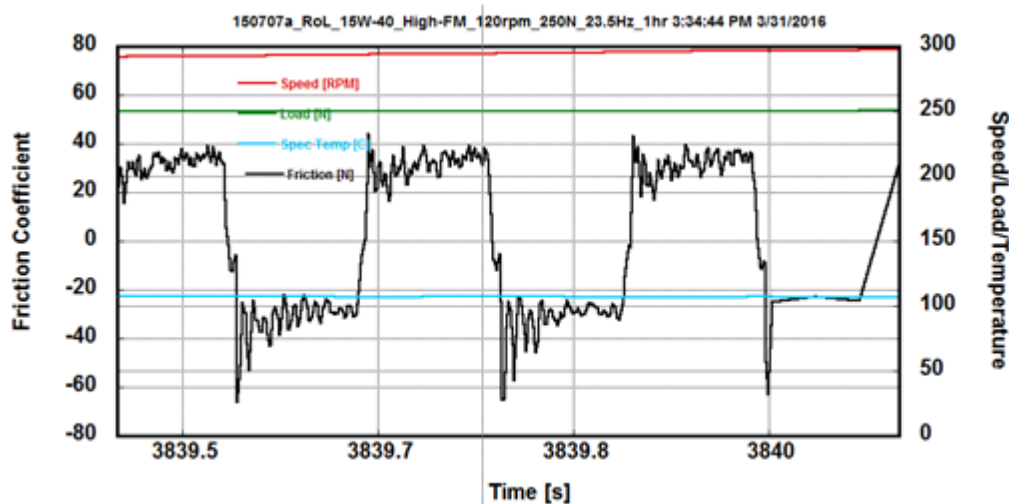


Figure 1. Friction as a function of time for a segment of time during test # 150707a (100 $^{\circ}\text{C}$).

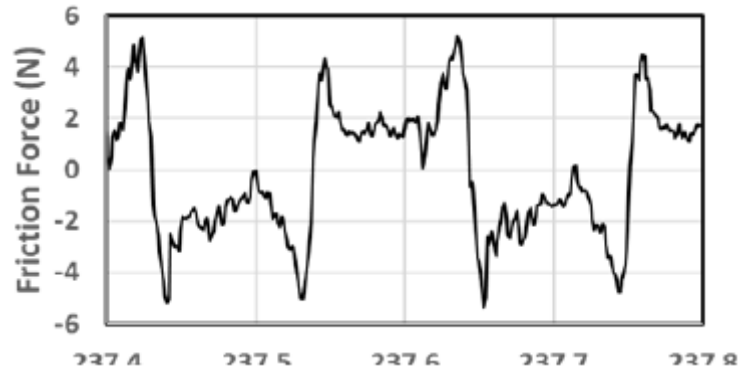


Figure 2. Friction as a function of time during a nominal room temperature run at 5 Hz (test # 150707c).

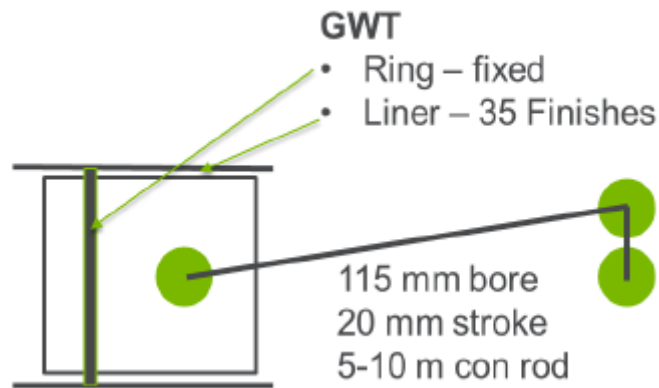


Figure 3. Ringpak model of AART benchtop tests.

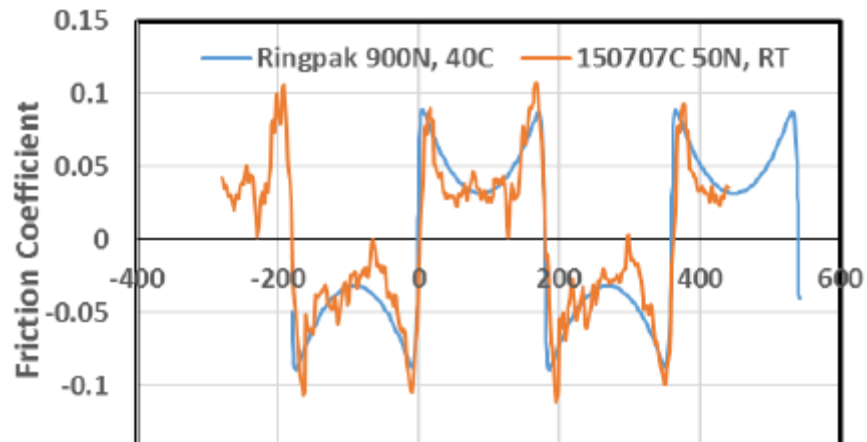


Figure 4. AART RINGPAK predicted and measured friction behavior for 150707C.

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AVPTA Technology Focus Area 4 Adjunct: Tire Efficiency

Improved Tire Efficiency through Elastomeric Polymers Enhanced with Carbon-based Nanostructured Materials

DOE-VTO TFA Lead: David Anderson
TARDEC TFA Lead: Dr. Jay Dusenbury

Principal Investigator:
Dr. Georgios Polyzos

Affiliation:
Oak Ridge National Laboratory (ORNL)
Oak Ridge, TN 37831-6054

Project Start: Q1FY16
Estimated Completion: Q1FY18

Objectives:

- Reduce hysteretic losses for reduction of rolling resistance
- Sharply enhance the wear resistance of the tire without compromising its viscoelastic properties.
- To uniformly disperse well-defined structures of self-assembled graphene layers in the rubber matrix
- 4% improvement in fuel efficiency

Strategic Context:

- Demonstrate a battlefield fuel reduction and reduce the logistics burden.
- Increase Power Density and Energy Efficiency resulting in increased vehicle range, endurance and operational tempo.
- Increase fuel efficiency of ground vehicles to Reduce Life Cycle Costs.
- Incorporate into Tactical Vehicles currently using commercial tires.
- Leverage technology to develop for military specific tires.

Accomplishments:

- Fabricated exfoliated graphene nanoplatelets with specific properties
- Synthesized silica nanofibers with diameter smaller than 100nm

Introduction:

In materials science of elastomers the influence of manufactured nanomaterial filler particles is of utmost significance for the performance of innovative rubber products, i.e., passenger and commercial tires with ultralow rolling resistance but high traction. Advances in both performance areas are imperative for the development of improved tire efficiency to meet Department of Energy's (DOE) fuel consumption reduction target of 4%, all while maintaining or improving wear characteristics of the tire. The unique geometrical configuration of the graphene fillers makes them the most promising carbon based fillers for breakthrough reduction of the rolling resistance.

Approach:

The approach capitalizes on the recent advances in nanomaterial and graphene synthesis and functionalization to suggest a promising avenue for the amalgamation of cutting-edge nanotechnologies that can be utilized towards DOE's technical targets. Recent research efforts focus mainly on the development of composite tires based on carbon black and silica. The project goal is to replace existing fillers (such as carbon black and silica) with higher performance materials (viz., graphene and silica nanofibers). At the conclusion of the project, the team will deliver prototype fuel-efficient tires and control tires. These tires will be evaluated at the Tank Automotive Research Development and Engineering Center (TARDEC). This project will be conducted in collaboration with Michelin Americas Research Company.

Results and Discussion:

Graphene flake aggregates were exfoliated in solution using high shear mixing and ultrasonic agitation to generate graphene nanoplatelets. (See Figure 1.)

Silica nanofibers with a diameter smaller than 100nm were synthesized in solution. (See Figure 2.) The diameter of the fibers were between 85-100nm. The silica nanofibers will be evaluated to demonstrate modulus values greater than 50 GPa.

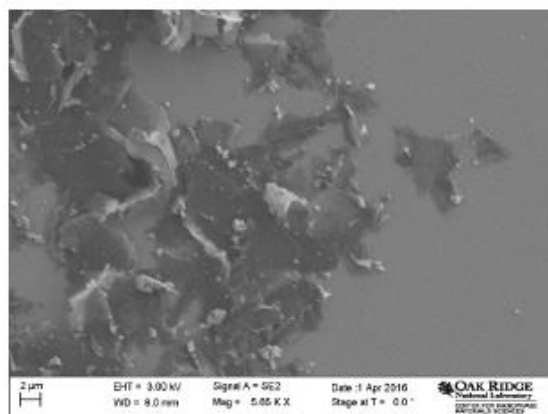
Conclusion:

High performance materials (Graphene and Silica Nano-fibers) were generated for this project. These filler materials will be evaluated for dispersion in the elastomer compound, with the goal to reduce hysteretic losses in the compound, and thus improve fuel efficiency.

Figures Begin on Next Page

Figures:

Graphene flake aggregates



Exfoliated graphene

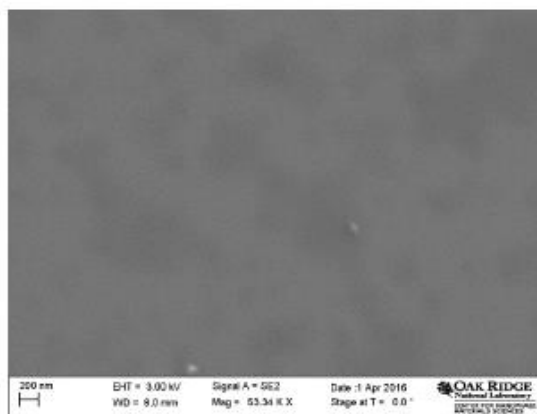


Figure 1. Exfoliation of Graphene Nanoplatelets

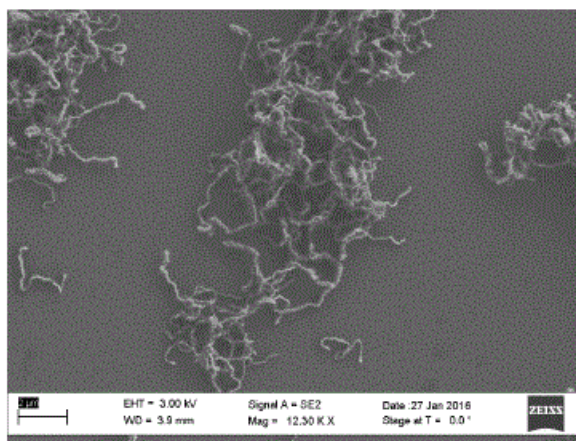
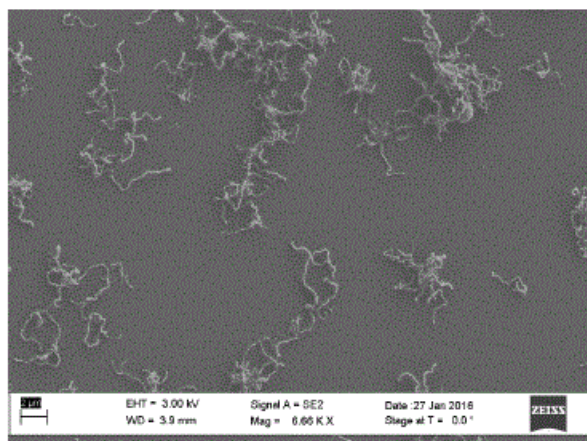


Figure 2. Synthetization of Silica Nanofibers

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AVPTA Technology Focus Area 4 Adjunct: Tire Efficiency

Advanced Truck and Bus Radial Materials for Fuel Efficiency

DOE-VTO TFA Lead: David Olett
TARDEC TFA Lead: Dr. Jay Dusenbury

Principal Investigator:
Dr. Lucas Dos Santos Freire

Affiliation:
PPG Industries, Inc
Monroeville Technical Center
440 College Park Drive
Monroeville, PA 15146

Project Start: Q1FY16
Estimated Completion: Q2FY18

Objectives:

- Develop a novel surface-modified silica technology and demonstrate 4-6% improved fuel efficiency of truck and bus radial (TBR) tires built from the technology.
- Proposed fuel efficiency increase will be achieved while maintaining or improving tear strength and tread wear.

Strategic Context:

- Demonstrate a battlefield fuel reduction and reduce the logistics burden
- Increase Power Density and Energy Efficiency resulting in increased vehicle range, endurance and operational tempo.
- Increase fuel efficiency of ground vehicles to Reduce Life Cycle Costs
- Incorporate into Tactical Vehicles currently using Commercial Tires
- Leverage technology to develop for military specific tires

Accomplishments:

- Determined surface energy of treated silicas and rubbers
- Directly observed the distribution of different fillers in binary polymer blends.
- Developed prototype silica fillers which show improved dispersion and lower tan delta values which correlate to lower rolling resistance.

Introduction:

Fuel-efficient silica fillers were adopted for passenger tires over 20 years ago. However, similar fuel-efficient benefits have not been realized for truck and bus radial tires. This project is focused on modifying silica to create an affinity for natural rubber as well as synthetic rubbers so that new, fuel-efficient truck and bus radial tires with optimized wear and tear properties result.

If half of the Class 8 vehicles on the road were to increase fuel efficiency by 4%, a potential 1.5 billion gallons of diesel, corresponding to \$5.8B and 15 million metric tons of CO₂ emissions, could be saved.

Approach:

This project begins with the team systematically and thoroughly investigating the properties that enable uniform dispersion of silica in both natural and synthetic rubbers. This knowledge will drive custom silica synthesis. Once novel silicas are developed that can be uniformly dispersed throughout multiple rubber types, the team will develop new TBR tread compound formulas. The formulas will be tested at bench scale to predict performance with the best performers being built in actual tires so that on-tire testing can be completed. Two rounds of formulation and tire builds will be conducted during the project to confirm viability. At the conclusion of the project, the team will deliver prototype fuel-efficient tires and control tires. These tires will be evaluated at the Tank Automotive Research Development and Engineering Center (TARDEC).

This project will be conducted in close collaboration with Bridgestone Americas Tire Operations. Bridgestone's technical lead is Dr. Amy Randall, Manager of Advanced Materials.

Results and Discussion:

Silica prototypes with low surface energy were developed with improved filler dispersion in natural rubber compound. (See Figure 1)

PPG also developed treated silica technology that demonstrated a 10% increase in dispersion in multiple rubber compounds compared to control carbon black or untreated silica technologies. Figure 2 shows the prototype silica disperses more uniformly between mixing phases in polymer blends.

Compound data generated from these silica prototype fillers used in polymer blends showed lower tan delta values (which correlates to lower rolling resistance) and higher tear resistance when compared to the control filler (carbon black) which is in line with the goals of the project.

Conclusions:

Prototype treated silica filler technologies were developed with higher dispersion for both single Natural Rubber (NR) and polymer blends (NR/SBR, NR/BR). These prototype fillers resulted in lower tan delta values, which is a laboratory indicator of lower rolling resistance (improved fuel efficiency).

Figures and Tables:

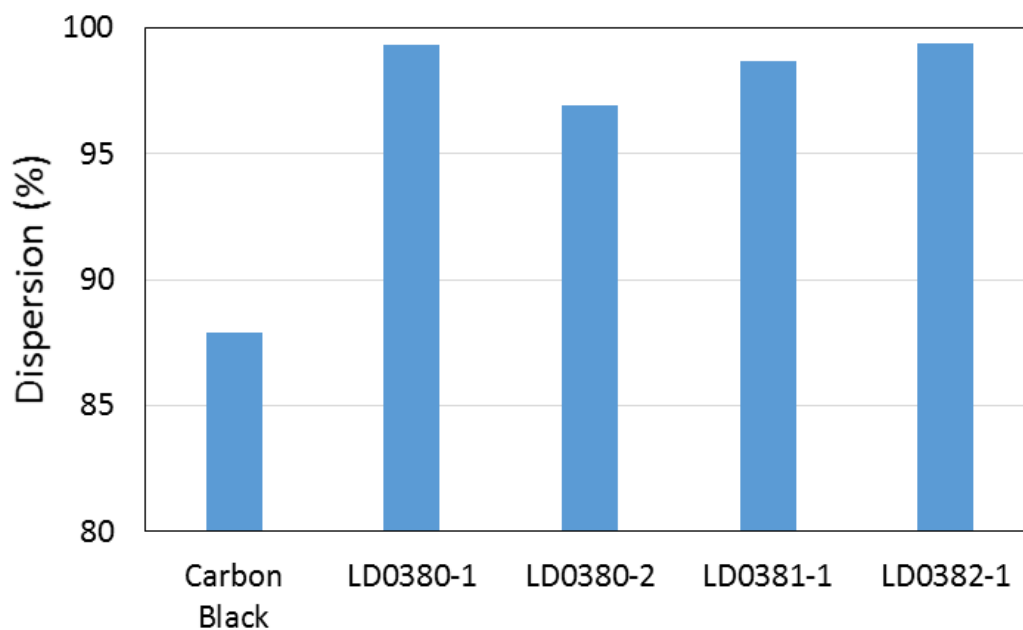


Figure 1. Dispersion in Natural Rubber (NR) Compound

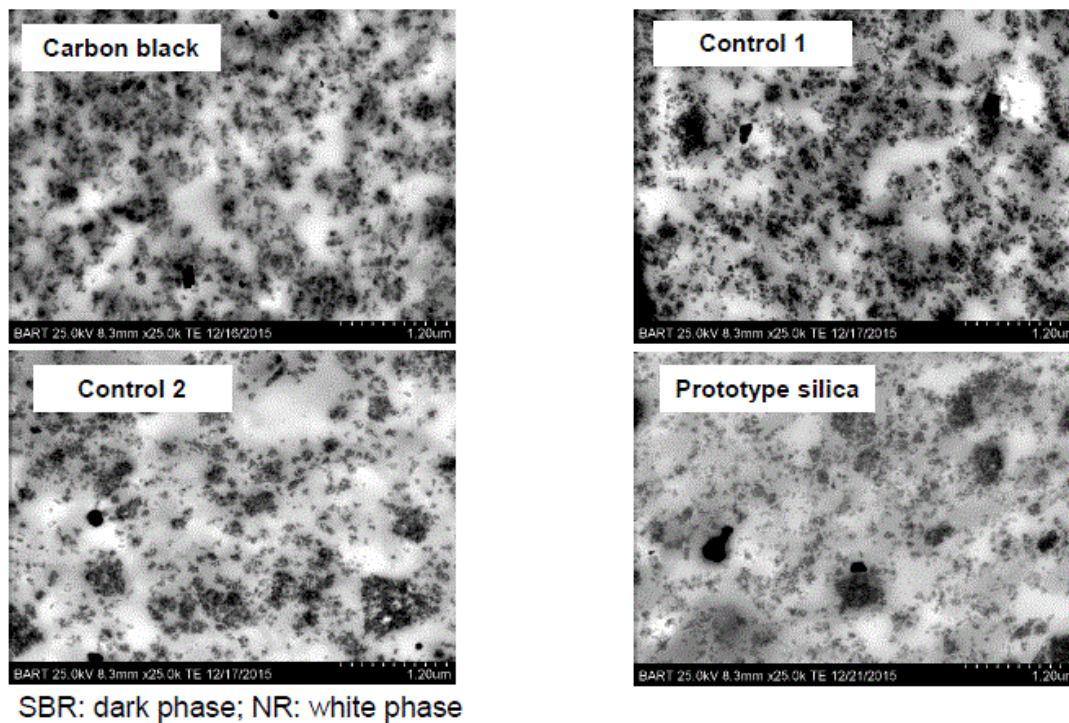


Figure 2. Dispersion in NR/SBR Polymer Blends

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AVPTA Technology Focus Area 5: Electrified Propulsion Systems

Non-Rare-Earth Integrated Starter Generator

DOE-VTO TFA Lead: Susan Rogers
TARDEC TFA Lead: Dean McGrew

Principal Investigators:
Joshua Tylenda, Joe Heuvers and Dean McGrew

Affiliation:
Ground Vehicle Power & Mobility
U.S Army TARDEC

Project Start: Q1FY13
Estimated Completion: Ongoing

Objectives:

- The TARDEC Advanced Propulsion Team, in collaboration with the DOE Vehicle Technologies Office, is working to develop and demonstrate two Integrated Starter Generators (ISG) without rare-earth permanent magnet materials suitable for onboard vehicle power generation.
- Most high-performance electric machines in hybrid electric applications use rare-earth magnets (NdFeB & SmCo) to achieve the required power and torque densities.
- This effort will additionally explore alternate electric machine topologies to achieve its goals.

Strategic Context:

Through the Non-Rare Earth ISG project, TARDEC's strategy is to develop the following:

- Ability of the motors to meet the specified performance without the use of rare-earth magnetic materials.
- Ability to perform according to schedule given issues and delays that have emerged.
- Ability to minimize audible noise signature of the Switched Reluctance (SR) generator topology.

To help manage risks, weekly status meetings are held to allow issues to be surfaced in a timely manner and mitigations put in place to resolve them in order to maintain schedule. Additional contract actions are planned to address audible noise of the SR topology.

Accomplishments:

- The Power Electronics & Electric Machinery Research group from Oak Ridge National Laboratory (ORNL) completed detailed design, controls and characterization testing for the baseline SR ISG with an inverter from Applied Power Systems (APS).
- The Spoke IPM design, controls and characterization testing was completed at Remy's facility in Anderson, IN with an inverter from American Traction Systems (ATS).
- The University of Akron replaced Remy as subcontractor to DCS for design, build and characterization testing of three novel design optimizations (*Tasks 3-5*) for reducing acoustic noise while maintaining target performance characteristics.
- *Task 3* SR ISG optimized design with windowing completed PDR and CDR and is currently in build.
- *Task 4* SR ISG optimized design with skewing completed PDR and CDR.

Introduction:

The Non-Rare-Earth ISG project has the opportunity to reduce the cost of high-performance power generation hardware. This project seeks alternatives to rare earth designs in case of a supply disruption of rare-earth permanent magnet materials similar to events in 2010-2011. In July 2010, China cut its exports rare earth minerals by 72%. In September 2010, China temporarily cut rare earth exports to Japan due to a maritime dispute. In 2011, China had cut exports further and raised export tariffs for rare earths. The world remains almost completely dependent on China for rare earths.

In 2010, The Department of Energy had published a Critical Materials Strategy, ranking Neodymium and Dysprosium among the most critical from an importance and supply risk perspective. Both materials are used in the highest performance Neodymium Iron Boron (NdFeB) permanent magnets available today.

Approach:

This project commenced with trade studies to identify the two most promising ISG architectures without rare-earth permanent magnets and to identify permanent magnet materials which could be leveraged for this effort. The two ISG architectures which were down-selected include the Switched Reluctance (SR) and Spoke Interior Permanent Magnet (Spoke IPM). The SR architecture does not include permanent magnets. The Spoke IPM is leveraging ferrite magnets which have approximately 1/10 the energy product of high performance rare earth magnets.

A study on permanent magnets revealed that ferrite and Alnico permanent magnets are the only non-rare-earth permanent magnets available in sufficient quantities to achieve the program goals. Due to the low coercivity of Alnico magnets, ferrite was determined to be the most promising choice for the design.

The SR ISG has emerged as the more promising of the two designs evaluated and now being built under the effort. The SR topology is more cost effective than any other known

generator architecture - approximately 1/3 the cost of comparable rare earth permanent magnet based designs.

Results and Discussion:

Performance projections for the two ISGs based on Finite Element Analysis are shown in Figures 5 and 6.

Tasks 1 & 2 were closed out, with SR ISG and Spoke IPM builds, optimizations and testing completed.

The Switched Reluctance (SR) ISG resulted in better performance, and was chosen for *Tasks 3-5* for building additional ISGs with optimization for reducing audible noise as identified in the trade study. *Task 3* optimized design through windowing in the stator and rotor. *Task 4* optimized design through skewing in the stator and rotor. These tasks have both successfully completed CDR, and will be built and tested against the baseline ISG during FY17.

Optimized control algorithms to reduce the audible noise of the SR ISG was completed with submission of PDR materials

Conclusions:

Contractor DCS identified the University of Akron to replace Remy as subcontractor to carry out *Tasks 3-5* for optimized designs and builds of the SR ISG. CDR has been completed for *Task 3 and 4* at the end of FY16.

Future Direction:

Build and validation of the *Task 3* windowed SR ISG will be completed during Q2FY17. Procurement of the *Task 4* skewed SR ISG build will start in Q1FY17. *Task 5* for a third novel design and build of an SR ISG will take place during Q3FY17. Each of three designs will be tested and characterized in comparison with the baseline machine built and delivered by Remy in terms of performance and acoustic noise reduction.

Figures and Tables Begin on Next Page

Figures and Tables:

	<i>Objective</i>	<i>Threshold</i>
<i>Machine Dimensions</i>		
Housing Outside Diameter	< 558 mm (22 inches)	
Overall Active Length	100 mm	120 mm
<i>Power Supply</i>		
Nominal Voltage:	600 V $\pm$ 35 V	
<i>Thermal Requirements</i>		
Liquid cooling	WEG / PWG	
Inlet Temperature	110°C	105°C
Cold Start Initial Condition	-50°C	
Maximum Flow Rate	< 30 LPM (8 GPM)	
Maximum Pressure Drop	16 PSI	
Operating Air Temperature	-50°C to 125°C	

Table 1. Technical Targets**Remainder of Page Intentionally Blank**

	<i>Objective</i>	<i>Threshold</i>
Target performance		
Continuous Power	100 kW	
Max Operating Speed	4250 RPM	3200 RPM
Base (corner) Speed	800 RPM	1100 RPM
Continuous Torque (0-800 RPM)	1200 Nm	
Peak Torque (0-800 RPM)	1800 Nm	
Duration of Peak Torque	30 sec	
Torque Density		
Volumetric Torque Density	80 Nm/L	50 Nm/L
Gravimetric Torque Density	11 Nm/kg	7 Nm/kg
Power Density		
Volumetric Power Density	8 kW/L	5 kW/L
Gravimetric Power Density	1.2 kW/kg	0.8 kW/kg

Table 2. Performance Targets

Other
Compatible with SAE#1 Bell-housing. Designed for integration between Caterpillar C9 engine and Allison 3200SP transmission.
Waterproof (per 3.5.1.2 from MIL-S-3785E(AT))
Conform to MIL-STD-461F (EMC)
Resolver control hall-effect redundancy

Table 3. Other Specifications

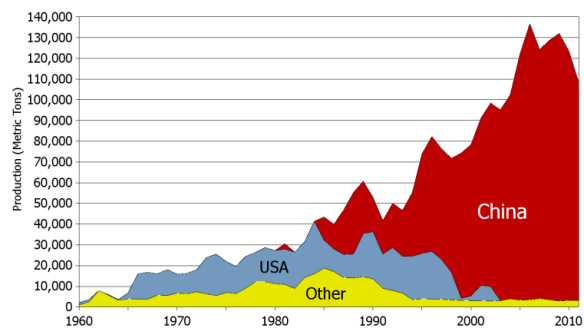


Figure 1. World-Wide Production of Rare-Earth Materials

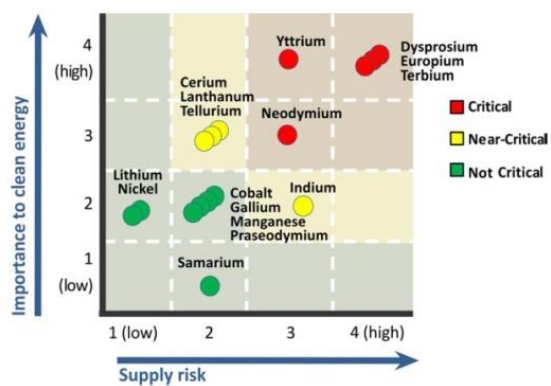


Figure 2. Department of Energy
Critical Materials Strategy

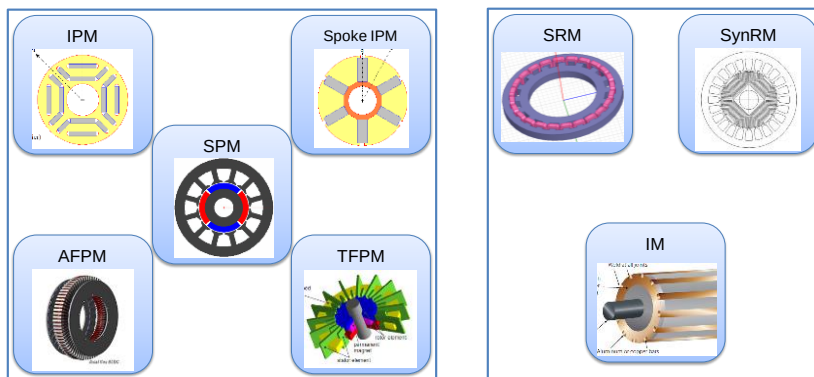


Figure 3. ISG Architectures

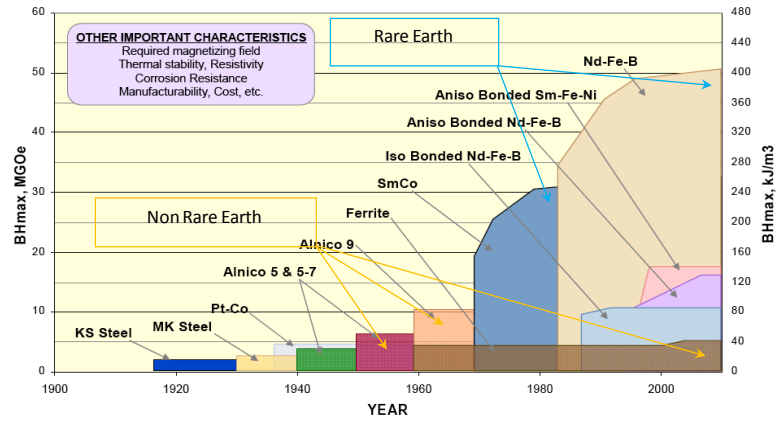


Figure 4. Non-Rare-Earth Permanent Magnet Quantities

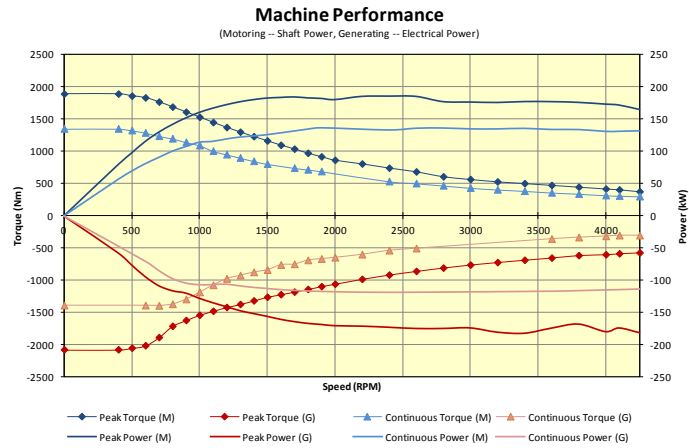


Figure 5. Characteristic Machine Performance

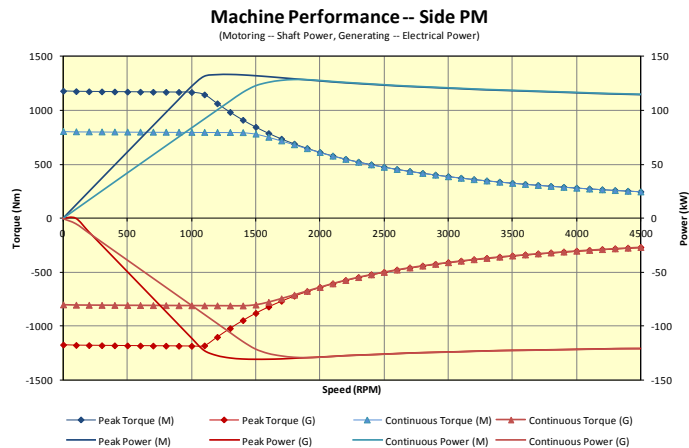


Figure 6. Side PM Machine Performance

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AVPTA Technology Focus Area 6: Energy Storage & Batteries

Efficient Safety & Degradation Modeling of Automotive Li-Ion Cells & Packs

DOE-VTO TFA Lead: David Howell
TARDEC TFA Lead: Dr. Laurence Toomey

Principal Investigator:
Dr. Christian Shaffer

Affiliation:
EC Power, LLC
341 N. Science Park Rd.
State College, PA 16803

Project Start: Q2FY13
Estimated Completion: Q1FY17

Objectives:

- Develop an efficient & robust pack-level safety model.
- Develop mechanism-based, fundamental models for accurately predicting degradation of Li-ion batteries under user-specified and wide-ranging temperatures and operating conditions;
- Perform co-simulation of our software with structural mechanics software via the Open Architecture Standard, developed by Oak Ridge National Laboratories;
- Perform testing and validate the cell and pack-level safety models and degradation models over wide-ranging temperature and operating conditions;
- Expand extensive materials database by experimentally characterizing and adding commercially-relevant cathode material, NCA, to our materials database.

Strategic Context:

- Key barriers to more widespread adoption of hybrid and electric platforms include challenges in the design of large-format Li-ion cells and packs related to performance, safety, life, and abuse.
- In this project, we are developing and refining commercial physics-based software tool that is directly aimed at helping cell manufacturers, the military, and automakers overcome these design challenges and barriers through an accurate and fast computer aided engineering tool.

Accomplishments:

- Completed cell and pack nail penetration tests
- Developed a nail penetration model and finished cell and pack model validation
- Completed cycle life tests of NCM111 and NCM622 cells for both high power and high energy types
- Developed a comprehensive cycle life model by incorporating the new crack formation-growth mechanism and completed model validation against four types of cells with both high power and high energy and two cathode materials, NCM111 and NCM622.
- Completed overcharge tests for both NCM and NCA cells
- Developed a new battery overcharge model and performed model validation against NMC/C cell data.

Introduction:

In this project we aim to accomplish: (1) battery pack safety and abuse conditions, and (2) advanced degradation/life simulation. In terms of pack safety simulation, we have extended our safety capabilities to include a truly deterministic pack model safety simulation, where the user inputs nail/short properties, location, nail speed, etc., for a cell in the pack, and can use the tool to investigate how the safety event propagates through the pack both thermally and electrochemically. Our end product is a truly deterministic pack safety model, whereby the user inputs a short location, short properties, nail speed, coolant type/properties, coolant flow rate, etc., and the electrochemical-thermal coupled model will simulate how the short propagates through the pack, both thermally and electrochemically.

We have also greatly extended our degradation models by incorporating the following processes: (1) as active material particles swell and shrink with lithiation, the particles crack with cycling, and (2) electrode structure degradation (ESD) occurs and how it depends on electrode loading or thickness. ESD hypothesis is that stress formation and development in thick electrodes will cause crack propagation in graphite particles. Lithium is lost due to formation of SEI layers on the newly cracked surfaces; see much more details in ref.[1].

Overcharge can occur if the control electronics of the battery management system (BMS) malfunction. It can also occur if there is severe cell imbalance in a battery pack. The thermal response of Li-ion cells during overcharge is largely determined by the cathode chemistry. Measurements of heat flow from the cells have shown that there is a rapid increase in heat generation when all of the lithium has been removed from the cathode. Overcharge may also cause plating of lithium in the graphitic anode, which not only leads to capacity loss but may also induce internal short-circuit due to the growth of lithium metal dendrite.

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Approach:

Nail Penetration Testing and Modeling:

Nail penetration of a single cell and multi-cell pack have been investigated both experimentally and theoretically in this project. Figure 1 displays the experimental setup where nail temperature is carefully measured. Figure 2 shows the numerical simulation setup for a 3-cell pack nail penetration and requisite mesh. A customized AutoLion3D code was developed to simulate cell and pack nail penetration.

Cycle Life Testing and Modeling:

Our new model of degradation starts from prediction of stress evolution during battery cycling, estimation of crack propagation and the ensuing area of newly exposed surfaces, and then followed by determination of loss of active cyclable lithium. This model along with previously developed SEI layer model and oxide film growth model gives rise to a comprehensive degradation model that can predict the electrode thickness effect on battery cycle life. Simultaneously extensive cycling tests have been performed to collect data for NCM111 and NCM 622 cells for model validation, as pictured in Figure 3.

Battery Overcharge Testing and Modeling:

Safety associated with Li-ion cell overcharge is a very important issue for HEV and EV applications. Tolerance to overcharge depends strongly on charge rate and battery chemistry, particularly the cathode chemistry. During charge, cathode oxide material is delithiated. Different cathode materials have different residual stoich of Li at 100%SOC, e.g. $\text{Li}_{0.0}\text{FePO}_4$ and $\text{Li}_{0.48}\text{Ni}_{1/3}\text{Co}_{1/3}\text{Mn}_{1/3}\text{O}_2$. Further removing Li from cathode material may result in crystallographic changes in structure, releasing a large amount of heat and leading to cell thermal runaway. Overcharge of Li-ion cell triggers complex reactions, such as electrolyte decomposition and gas evolution, further leading to heat and pressure build-up within the overcharged cell. The present work simulates thermal and electrochemical consequences of overcharge where the heat generation data are taken from Sadia National lab's high quality tests (Ref.[2]). The voltage response is simulated without considering ensuing side reactions such as electrolyte decomposition and gas evolution.

The experimental setup for all overcharge tests is shown in Figure 4.

Results and Discussion:

Nail Penetration Testing and Modeling:

A representative comparison between the experimental and simulated temperature rise during nail penetration of a 3-cell pack is shown in Figure 5. It can be seen that the temperature peak is accurately captured; however, the time constant in reaching the temperature peak differs somewhat. Much more validation against extensive test data was performed, and overall good agreement between the experiments and simulations is achieved.

Cycle Life Testing and Modeling:

A representative comparison of the model prediction with charge-discharge performance at the beginning of life is shown in Figure 6. Excellent agreement is found under a wide range of operating conditions. Figures 7 and 8 depict experimental validation of the new degradation model against NCM622/C high energy and high power cell data, respectively. Again, good agreement is achieved in cycle life model validation. Much more validation is also performed for NCM111/C cells.

Battery Overcharge Testing and Modeling:

Preliminary validation of the presently developed overcharge model is performed against Sandia National Lab's test data (Ref.[2]) for three different cathodes: LFP, NCM and NCA. As can be seen from Figure 9, good agreement in cell temperature is achieved between experiment and simulation. Figure 10 compares measured and predicted cell temperature and voltage evolutions of a 2Ah NCM/C 18650 cell undergoing overcharge at 1C rate and 45°C. Again, overall good agreement is seen. It can be seen that cell voltage gradually increases before 90% of lithium (cathode stoich $\approx 10\%$) is removed from cathode, then it rises sharply to reach a peak of 5.1V when the current interrupt device (CID) is triggered. Not all the lithium can be removed from the cathode during overcharge^[3]. Further overcharging at higher voltage after stoich $\approx 10\%$ causes electrolyte decomposition and gas evolution, thus rapid temperature rise due to exothermic reactions. The current interrupt device (CID) is triggered by the pressure buildup inside the cell due to gas evolution. Before cathode stoich $\approx 10\%$, the predicted cell voltage matches the experimental data very well. The large discrepancy occurs only after stoich $\approx 10\%$, since high-voltage ($>4.8\text{V}$) electrochemistry is unknown and electrolyte decomposition and gas evolution are not included. The predicted temperature is also in good agreement with the measured data.

Conclusions:

In FY 2016, we have accomplished the following milestones:

- Completed cell and pack nail penetration tests
- Completed development of a nail penetration model and finished cell and pack model validation
- Completed cycle life tests of NCM111 and NCM622 cells for both high power and high energy types
- Developed a comprehensive cycle life model by incorporating the new crack formation-growth mechanism and completed model validation against four cells with both high power and high energy types and two cathode materials, NCM111 and NCM622.
- Completed overcharge tests for both NCM and NCA cells
- Developed a new battery overcharge model and performed model validation against NMC/C cell data

The project is on schedule and to be completed in March 2017. Our customized code based on the above-mentioned expanded capabilities is being used by defense and aerospace industries.

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1. X-G. Yang, C. Bauer, and C.Y. Wang, Journal of Power Sources, Vol. 327, pp. 414-422 (2016).
2. E. P. Roth and C. J. Orendorff, The Electrochem. Soc. Interface: summer 2012, 45 (2012).
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Figures:

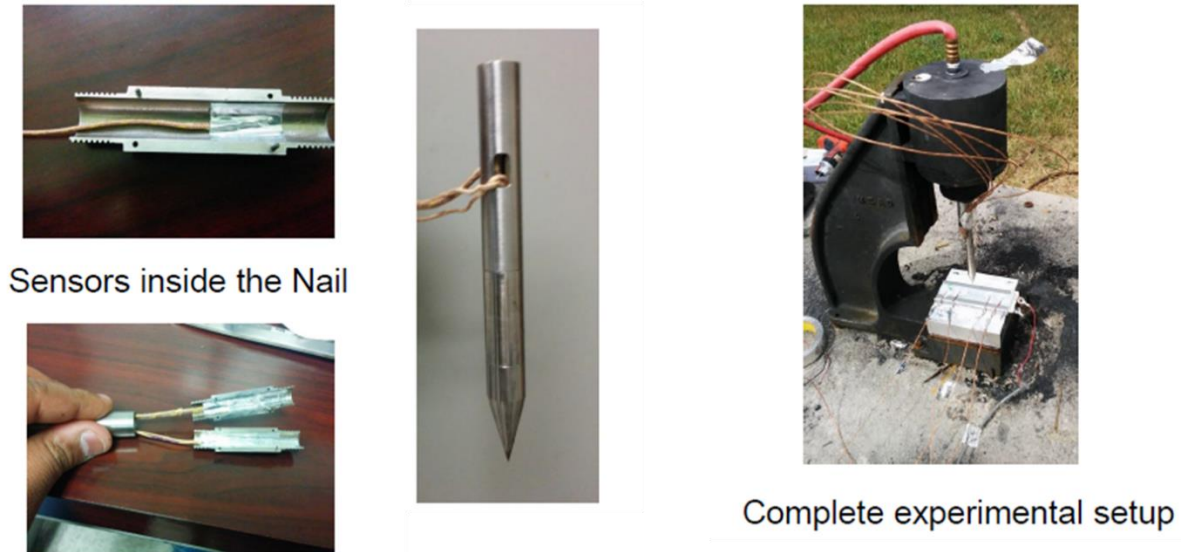


Figure 1. Cell/pack nail penetration setup

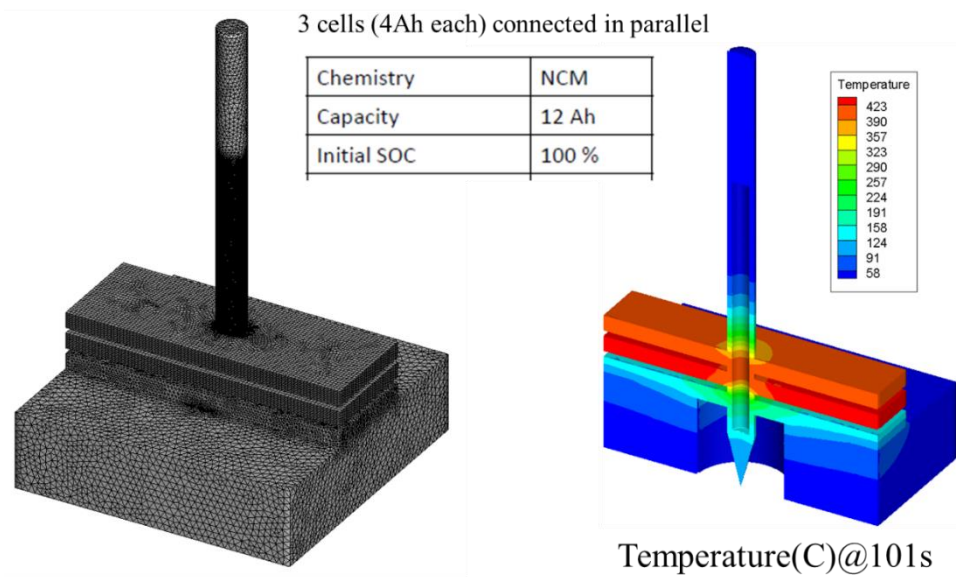


Figure 2. Nail penetration mesh setup and simulation results for a 3-cell pack

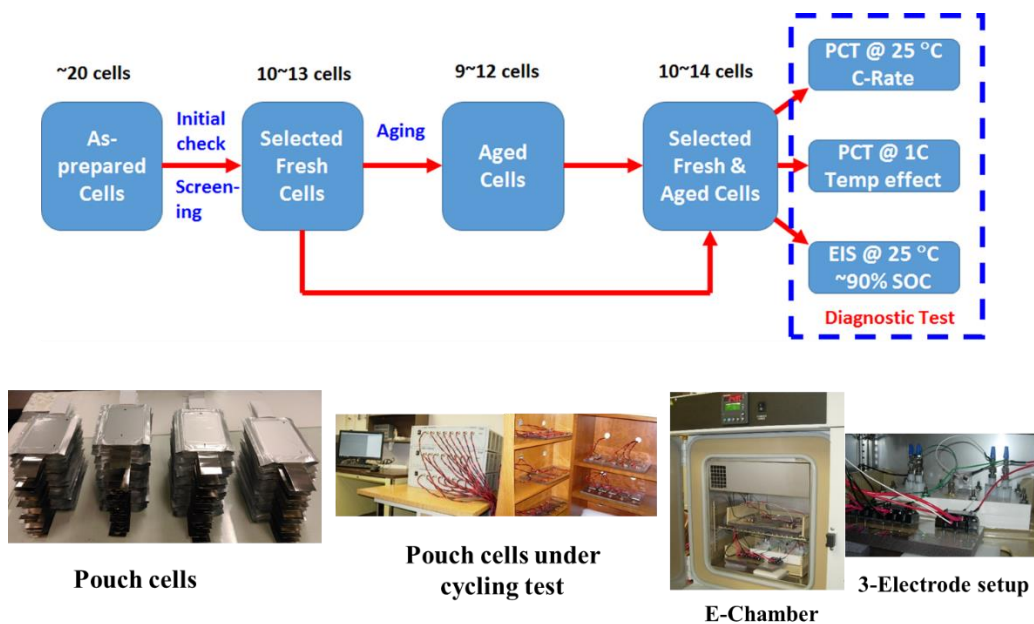


Figure 3. Experimental procedures for cycle life studies

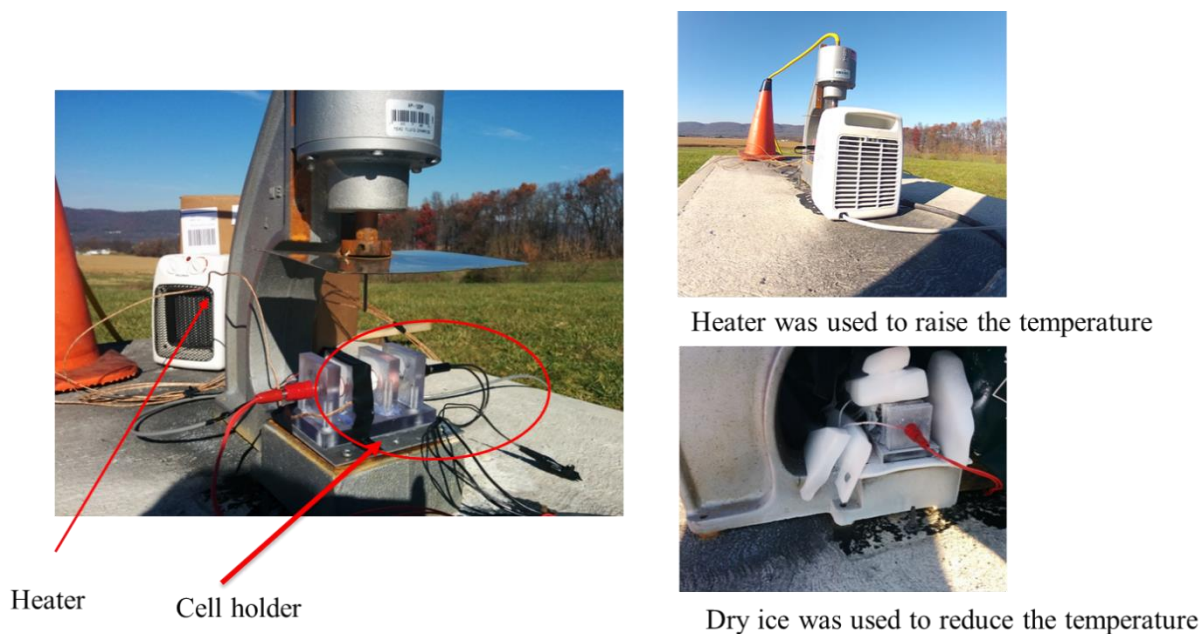


Figure 4. Experimental setup for battery overcharge testing

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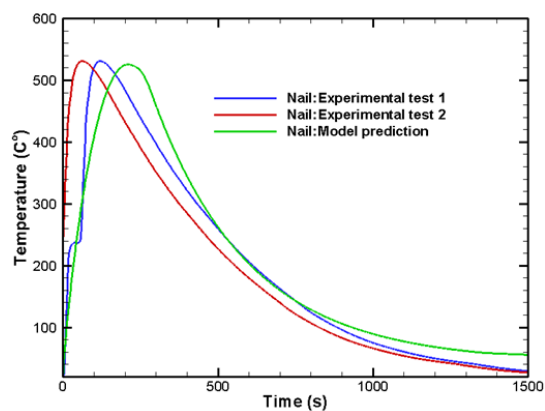


Figure 5. Experimental-model comparison of the nail temperature during a 3-cell pack penetration

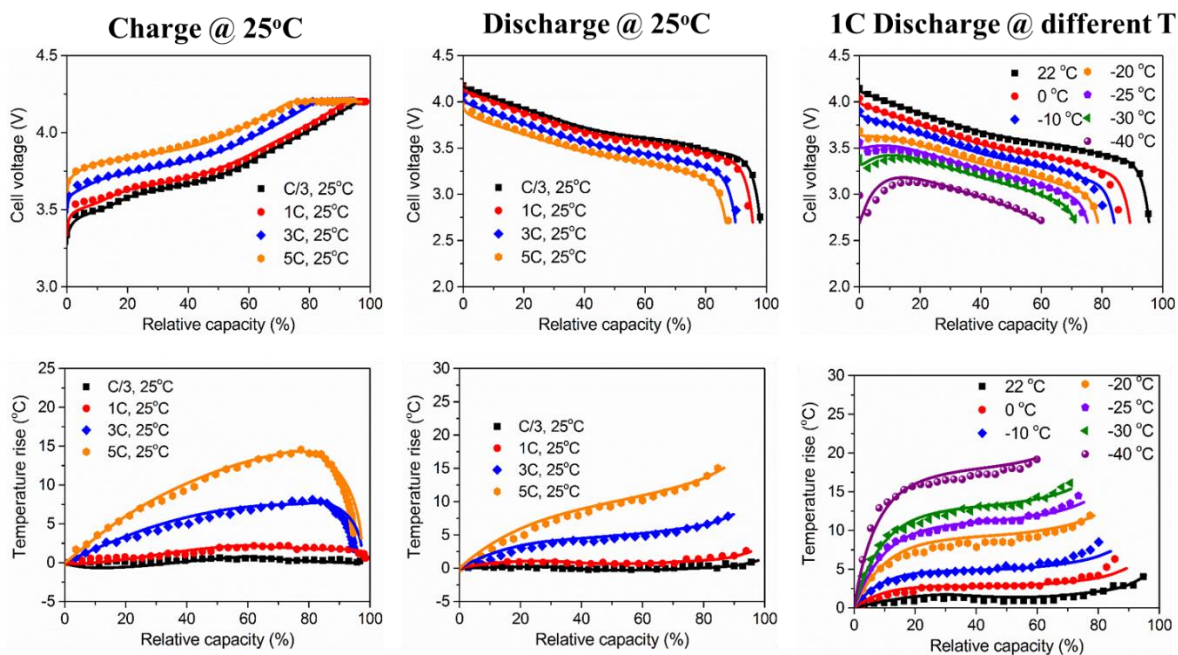
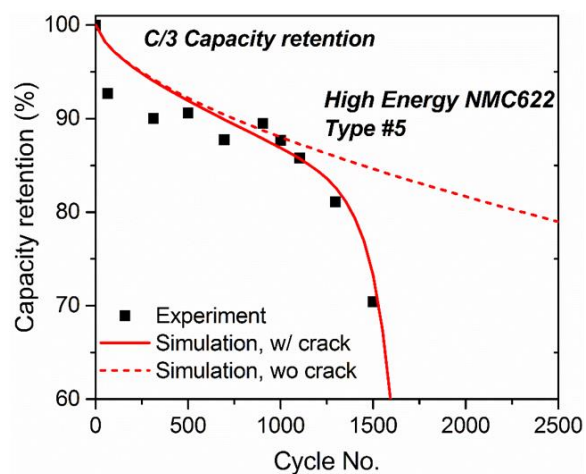
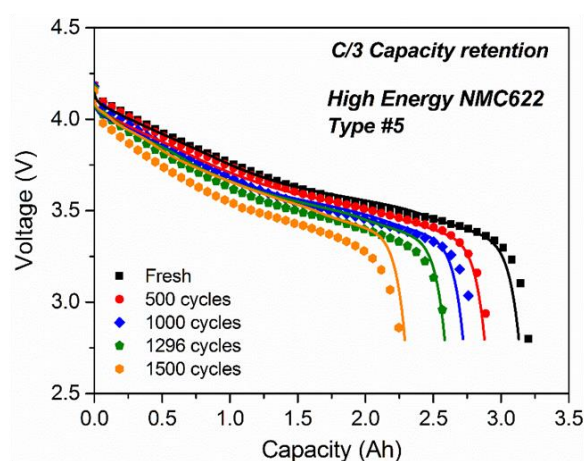


Figure 6. Experiment-model comparisons of beginning of life (BOL) performance for NCM622/C high energy cells (200 Wh/kg). Lines are model predictions, and symbols are experimental data.

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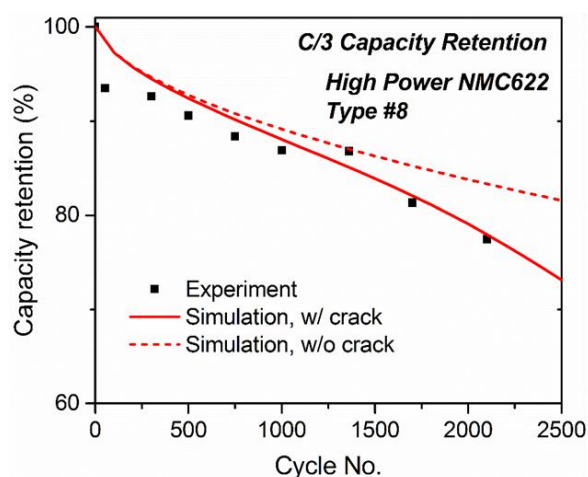


C/3 Capacity Retention

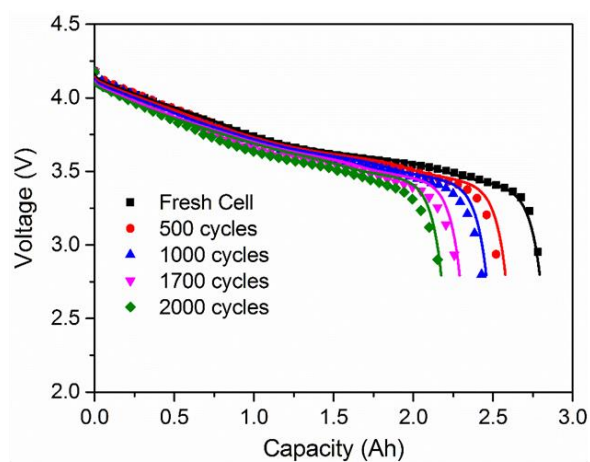


C/3 Discharge curve after various cycles

Figure 7. Experimental validation of degradation model for NCM622/C high energy cells (200 Wh/kg).



C/3 Capacity Retention



C/3 Discharge curve after various cycles

Figure 8. Experimental validation of degradation model for NCM622/C high power cells (165 Wh/kg)

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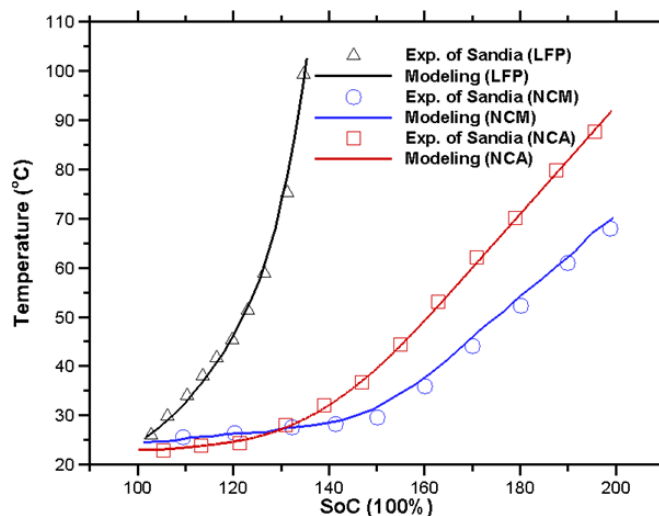


Figure 9. Experimental validation of battery overcharge model against Sandia National Lab's data (ref.[2]) for LFP, NCM and NCA cathodes.

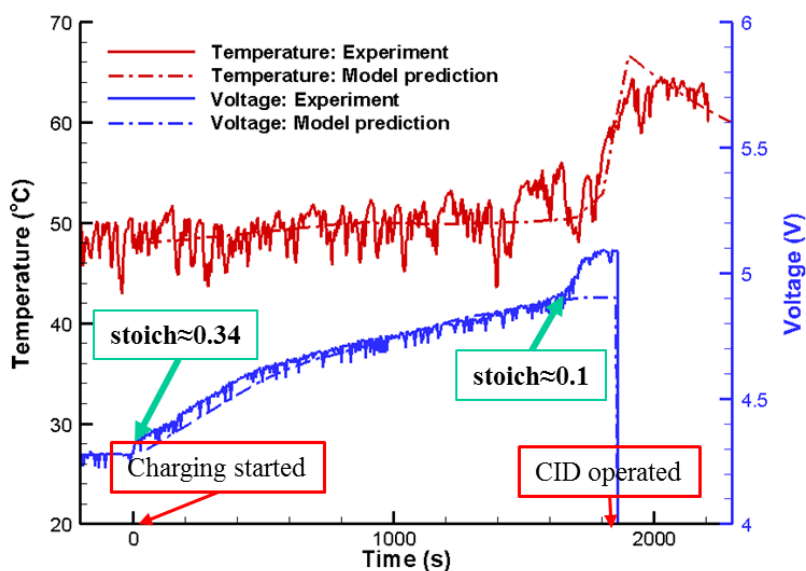


Figure 10. Experimental validation of battery overcharge model for a 2 Ah NCM/C cell under 1C overcharging and 45°C.

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AVPTA Technology Focus Area 6: Energy Storage & Batteries

Multi-physics Computer-Aided-Engineering Tools for Performance, Life, and Safety Analysis of Li-Ion Battery Systems in Military Vehicle Applications

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TARDEC TFA Lead: Dr. Laurence Toomey

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Project Start: Q2FY13
Project Completed: Q1FY16

Objective:

- The objective of the project is to develop a computational methodology for a significant enhancement in computation speed of nonlinear multiscale modeling of plug-in electric vehicle (PEV) batteries while maintaining or improving the solution accuracy from the most advanced state-of-the art models.

Strategic Context:

- The energy efficiency and functionality of military vehicles through electrification can be improved with energy storage system utilizing lithium-ion battery technologies. For engineering design, there is a lack of high-fidelity, fast-running simulation tools that correctly capture the physics of Li-ion batteries. In this project, NREL's multiscale multi-domain (MSMD) battery model is reformulated in a quasi-explicit framework that avoids time consuming nested iterations when solving models at different length scales. The method is demonstrated to be compatible with commercial battery and vehicle thermal simulation software tools, for broader dissemination in the battery and vehicle design community.

Accomplishments:

- Developed GH-MSMD, a new quasi-explicit, modular, extendable, tightly coupled, nonlinear framework in both the C++ and MATLAB platforms.
- Demonstrated that the new GH-MSMD speeds up computations by 1,000 times.
- Demonstrated implementation of GH-MSMD cell-domain model (CDM) in ANSYS/Fluent

- Built a custom graphical user interface (GUI) in ANSYS/Fluent for GH-MSMD simulation pre-processing.
- Compared options for an adaptive time-stepping algorithm in GH-MSMD versus the existing recursive method.
- Developed, validated and benchmarked an adaptive state variable model (A-SVM) of electrode-level dynamics as a new reduced-order model (ROM) option for MSMD
- Demonstrated that the A-SVM achieved 50x speed-up with accuracy better than 15 mV.

Introduction:

NREL pioneered the multiscale multi-domain (MSMD) model, overcoming challenges in modeling the highly nonlinear multiscale response of battery systems. The MSMD provides high extent flexibility and multi-physics expandability through its modularized architecture, as well as computational efficiency. However, further improvement of computational speed of the model is greatly desired to promote the application of the high fidelity multi-physics model in various battery engineering problems. In this project, we significantly improve the computation speed and stability of multiscale model framework by eliminating several layers of nested iteration through innovative multiscale coupling methodology, while still keeping the modular framework architecture, and provide a new reduced order model (ROM) that is adaptive to system evolution and identifiable with fewer compound parameters.

Approach:

The project target is achieved through complementary parallel efforts in framework efficiency improvement and component efficiency improvement. We developed a new quasi-explicit nonlinear multiscale model framework, GH-MSMD, using time-scale separation, variable decomposition, and partial linearization procedures. GH-MSMD eliminates several layers of nested iteration, significantly improve the speed and stability upon the original MSMD, and retain the modular framework architecture that is critical to battery behavior simulations. We also develop advanced ROMs for the component models. Computational time is often invested in advance to find a reduced order basis in a much lower dimension than that of the full ordinary differential equation systems derived from spatial discretization of the partial differential equation systems. The ROM basis is typically restricted to reuse in the system where its characteristics are evolving, such as the battery aging process. In this project, we developed the A-SVM, a new ROM that adapts to system evolution and identifiable with fewer compound parameters. For enhancing usability of the model, we constructed the MSMD-Fluent application programming interface for multi-physics integration of NREL's custom model library in a commercial software environment – ANSYS/Fluent.

Results and Discussion:

The following progress was achieved:

New Model Speeds Up Computations by 1,000 Times:

In FY14, NREL met the 100-fold computational speed-enhancement target for its MSMD model one year ahead of schedule. In FY15, we significantly exceeded the projected target by further improving the code structure and by extending the model to a larger scale. In FY16, we

demonstrated application of the cell-level GH-MSMD model approach in ANSYS-Fluent, proving the relevance of the method in a commercial battery/vehicle simulation software tool widely used by designers.

Figure 1 presents the comparison of the electrical and thermal response of a battery for a mid-size sedan plug-in hybrid electric vehicle (PHEV10) on the US06 20-minute driving power profile. While the model outputs are shown to be very close to each other, the new quasi-explicit, modular, extendable, tightly coupled, nonlinear MSMD framework, GH-MSMD, demonstrates that the most efficient electrode-scale battery-cell model option can run a 1,200-second driving profile simulation in only 0.74 seconds using a personal computer—an approximate 1,000-fold improvement over previous capabilities. In contrast, the original MSMD runs the same simulation in 654 seconds. When the model is extended to its full-scale, three-dimensional, larger cell domain, the speed-enhancement factor reaches 1,000 to 10,000, depending on the choice of sub-model.

Figure 2 compares the model solution variables in each computational domain and the coupling variables exchanged between the adjacent length scale domains in MSMD (left) and in GH-MSMD (right). Even though the solution algorithms are significantly different between the two, the model structures are similar. This comparison signifies the modularity of model framework that the GH-MSMD inherited from the MSMD. The new GH-MSMD framework retains the flexibility needed for application to various lithium battery chemistries and designs. It still integrates a sophisticated particle model to address particulate morphology, size distribution, surface modification, contact resistances, and mixture composition of active particles. The model simulates all major cell form factors with variable electrode compositions and designs.

Reduced Order Electrochemical Model Becomes Adaptive:

NREL developed a fast, accurate realization of the Newman electrochemical model that runs 100 times faster than typical numerical solutions in modern commercial software. Although spectral model order-reduction techniques are available to achieve speed enhancement, previous efforts that applied these methods for battery simulation required a cumbersome preprocessing step to identify the reduced model versus a few selected parameters of interest. To overcome this limitation, NREL eliminated the preprocessing step so that a simulation could run immediately, and fully populated the ROM look-up tables so that it is extendable to all possible lithium-ion porous electrode designs and states of health. The new A-SVM was validated and benchmarked against other EDM MSMD models (two MSMD-EDMs and two GH-MSMD-EDMs) in MATLAB. The compared MSMD EDM combinations are edLPD/pdPLLM, edPLM/edLPD, edSEG/pdPLM, and edSEG/pdSEG. Figure 3 presents the model output comparisons for a 5C and 10C pulse profile and constant current discharge in 1, 2, 5, and 10C. Accuracy is generally greater than 99%, and the speed-up factor of A-SVM against the highest-order segregated solver option is about 50. The unconditional stability of A-SVM enables a large time-step size, and additional speed-up is expected in practical situations. A-SVM shares the common input and output file structure with the MSMD/GH-MSMD. This achievement is expected to further enable computer-based optimization of lithium-ion cell designs and support computational simulation of battery degradation and aging.

Efforts to Promote Industry Access to New Models:

The successful development of GH-MSMD is expected to shift the paradigm in using a model for electric-drive vehicle battery system design and evaluation, potentially revolutionizing the standard development process for the entire industry. NREL's GH-MSMD baseline model codes are developed in both the MATLAB and C++ platforms. These NREL custom models are planned to be available to external users in the future. In the meantime, it is desired to implement GH-MSMD in commercial computer-aided engineering software to make it available immediately to a large number of users in the electric vehicle industry. In this regard, NREL developed a manual procedure for GH-MSMD implementation in ANSYS Fluent and built a GUI using scheme programming and user code. Figure 4 is a captured image of NREL's custom GUI of GH-MSMD. The current GUI is similar to that in the ANSYS/Fluent MSMD Battery Module. The customized GUI enables us to practice and test GH-MSMD implementation into Fluent. Unique features could be added for the GH-MSMD methodology to link different domain levels and improve simulation efficiency. NREL's implementation of the GH-MSMD CDM in Fluent has been verified by comparing the model outputs against the commercially available and existing MSMD model option in Fluent. The results are shown in Figure 5.

Conclusions:

We successfully accomplished the project goal and improved the computation speed of state-of-the-art nonlinear multiscale battery model by a factor of 100 while maintaining its solution accuracy. The new GH-MSMD demonstrates a 1,000-fold speed up compared with the original MSMD during vehicle driving profile benchmark simulation tests. Several remaining challenges and the future directions that we expect to address in future CAEBAT projects are identified below.

GH-MSMD demonstrates significant speed up. The remaining challenge, however, is to enhance the applicability of the new model to various battery engineering problems. We are working to summarize the GH-MSMD principles and implementation and publicize them to encourage contributions from outside experts. Under new projects initiated in FY16, we completed a journal article, now under review, on the GH-MSMD method and started working with ANSYS/Fluent to implement the method in their commercially available software platform.

To make the models more widely useful in industry, interdisciplinary constituent models relating material/ design/ process/ operational parameters with physicochemical parameters of the GH- baseline models are needed. We will develop sequential optimization procedures to break the under-determined parameter estimation problem of the whole system into a sequence of fully determined fits to subsets of the parameters and advanced model-based battery characterization.

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2. G.-H. Kim, C. Yang, A. Pesaran, "Integrated Multiscale Multiphysics Modeling of Dynamic Short Circuit Behavior in Large Lithium-ion Batteries," 228th Electrochemical Society Meeting, October, 2015, Phoenix, AZ.

3. C. Yang, G.-H. Kim, M. Keyser, A. Pesaran, "Numerically Characterizing Nail Penetration Testing for Safety Evaluation of Li-Ion Cells," 228th Electrochemical Society Meeting, October, 2015, Phoenix, AZ.
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Gi-Heon Kim, Kandler Smith, Jake Lawrence-Simon, Chuanbo Yang, "Efficient and Extensible Quasi-Explicit Modular Nonlinear Multiscale Battery Model: GH-MSMD," submitted (Sept. 2016)

Figures:

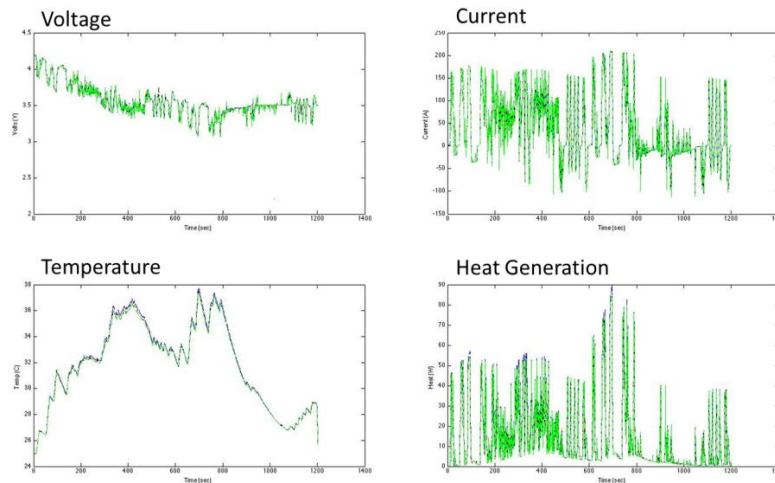


Figure 1. Comparison of Electrical and Thermal Response of a Battery for a Mid-Size Sedan Plug-in Hybrid Electric Vehicle (PHEV10) on the US06 20-minute Driving Power Profile from the GH-MSMD and the original MSMD.

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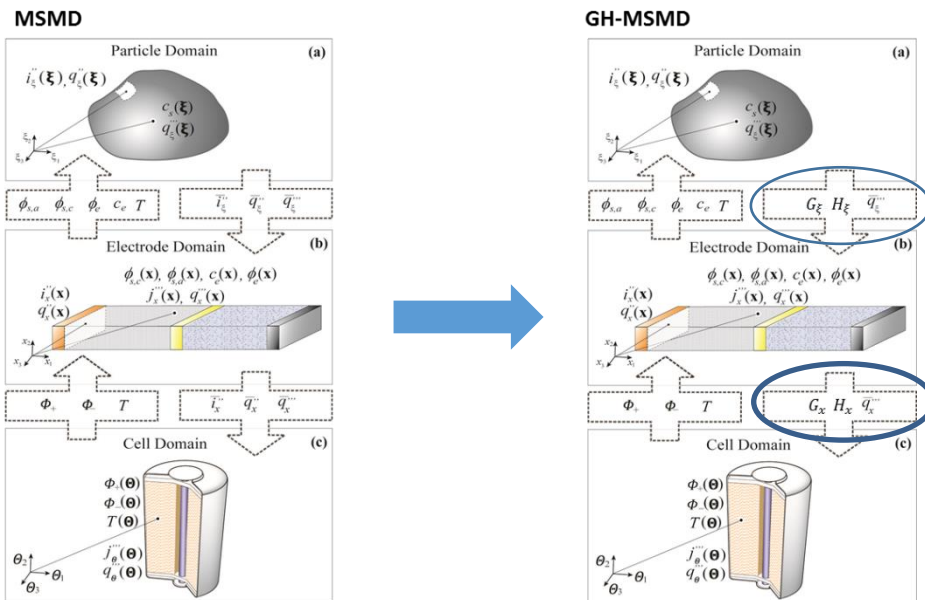


Figure 2. Comparison of the Original MSMD and the GH-MSMD Framework Structure and Main Changes in the GH-MSMD.

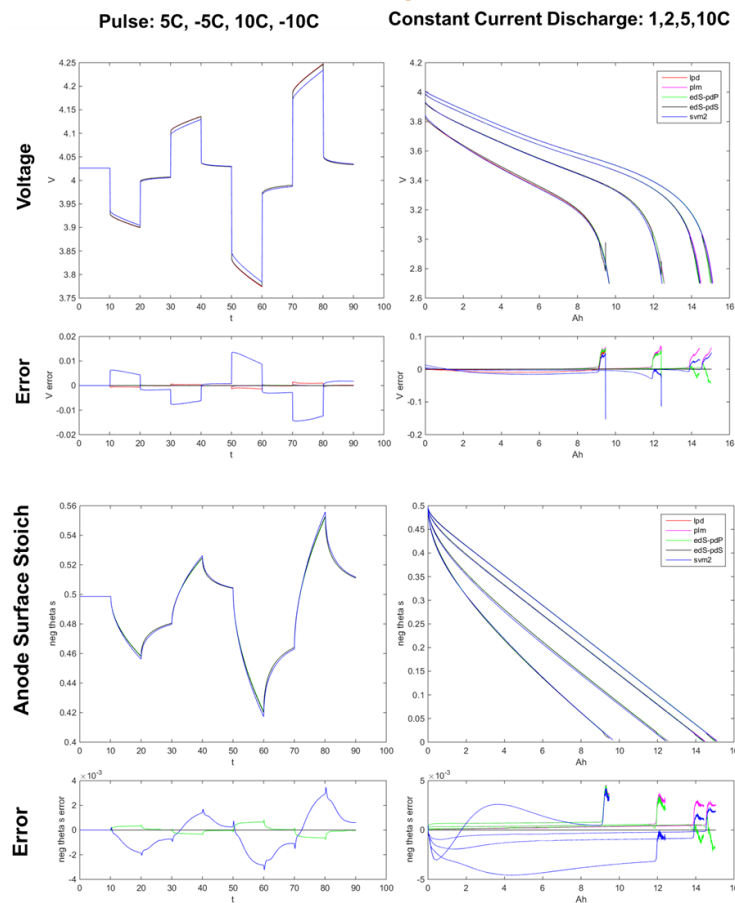


Figure 3. A-SVM Verification and Benchmark Results Against Various MSMD/GH-MSMD Models.

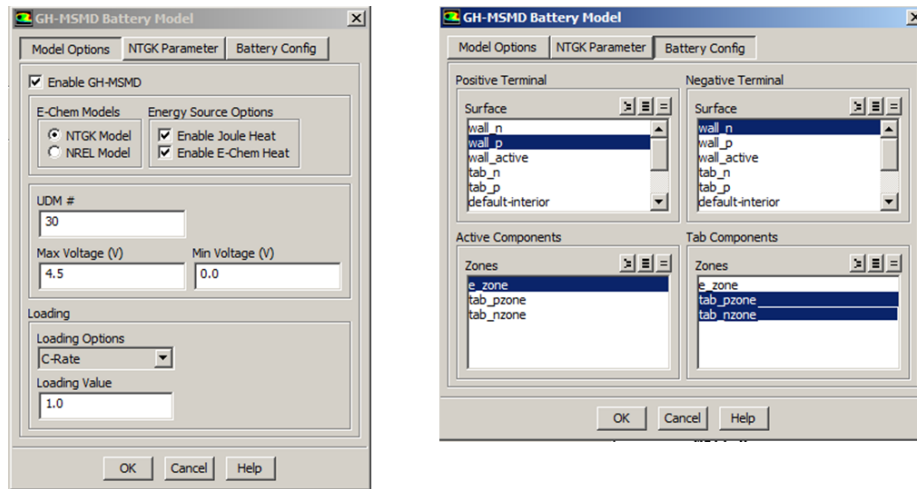


Figure 4. Custom GUI of GH-MSMD set up in ANSYS/Fluent

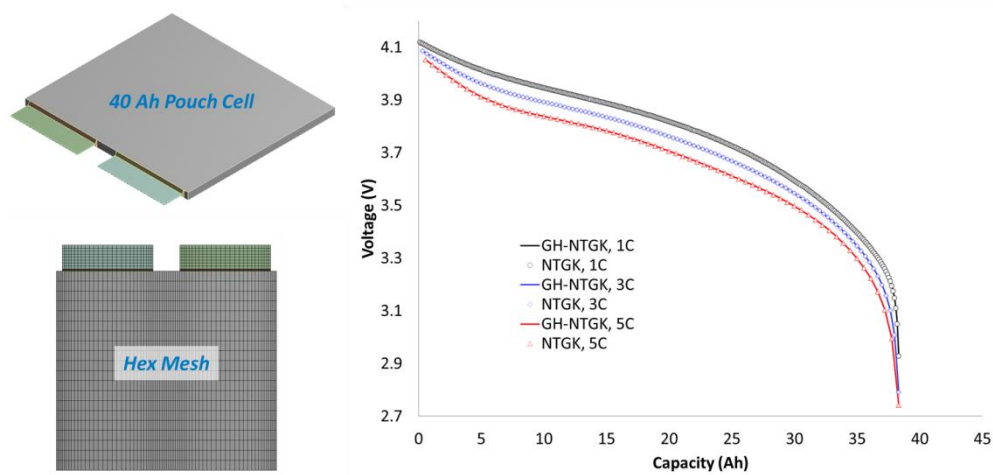


Figure 5. NREL's Custom Implementation of GH-MSMD in Fluent is Verified. Solid Lines are the Cell Voltage Response of NREL Custom GH-MSMD Model Simulations, and the Symbols are Corresponding Outputs from the Fluent MSMD Battery Simulation Module.

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AVPTA Technology Focus Area 6: Energy Storage & Batteries

Beyond Li-Ion: Overcoming Interface Impedance in Solid-State Batteries

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TARDEC TFA Lead: Dr. Laurence Toomey

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Project Start: Q2FY14
Estimated Completion: Q4FY17

Objective:

- Develop a multifaceted and integrated experimental and computational approach to solve the key issue in solid-state Li-ion batteries (SSLiBs), interfacial impedance. The research will focus on Garnet-based solid-state electrolytes (SSEs), but the knowledge can be applied to other SSE chemistries. The interfacial impedance in this proposal includes charge transfer, ionic and electronic transport, and interfacial structural/chemical stability over charge-discharge cycling. The developed low interface technique will be tested with solid state Li-NMC cell and Li-S cell testbeds that have 350-450 Wh/kg and 200 cycles.

Strategic Context:

- Generate a leap-ahead technology used for military vehicles to support the future power for TARDEC and the Army by enabling the development of advanced battery systems with significant increases in energy density
- Improve Battery safety characteristics to support vehicle silent watch and enable other high energy requiring applications.

Accomplishments:

- Identified compositions of Gel electrolyte to achieve $100 \Omega \cdot \text{cm}^2$ (Q1FY16 Milestone)
- Determined interfacial impedance in layered and 3D controlled solid state structures (Q2FY16 Milestone)
- Developed computation models to investigate interfacial ion transport with interlayers (Q3FY16 Milestone)

- Identified compositions of interlayers and processing with electrolyte/electrode interfacial impedance of $\sim 10 \Omega \cdot \text{cm}^2$ (Q4FY16 Milestone and Budget Period Go/NoGo)

Introduction:

Solid state garnet-electrolyte lithium ion batteries have tremendous potential due to their inherent safety, high voltage stability, and reasonably high conductivity. However, the interfacial impedance between solid state electrolytes and electrode is currently too high. This work will focus on reducing the interfacial impedance, by making controlled structures on the garnet electrolyte surface, and introducing conductive and conformal interfacial layers between the garnet and the electrodes. These results will address the primary issue and significantly advance solid-state Li-battery technology.

Approach:

The objectives outlined above will be accomplished by optimizing the garnet surface structure and electrode material, and investigating high conductivity conformal interfacial layers.

Effect of Interfacial Structure on Impedance:

While we and others have made tremendous advances in understanding interfacial resistance in solid oxide fuel cells (SOFCs), to date no one has applied these techniques to SSLiBs. Therefore, we use SOFC techniques to develop a fundamental understanding of interfacial impedance in terms of intrinsic charge transfer rates, ionic and electronic transport, and effect of interfacial structure.

Electrochemical impedance spectroscopy (EIS) of solid electrolyte and electrode or interfacial layer pellets are being performed to identify the mechanistic frequency dependence of EIS response for each material as well as blocking electrode and DC measurements to separate out ionic vs. electronic conductivity for each material. Then bilayer electrolyte and electrode/interfacial layer pellets with smooth and controlled interfaces are being fabricated and tested with EIS.

This allows for determination of the specific interfacial impedance, as it will be resolved as an additional EIS frequency response. This interfacial impedance is then being used to calculate the charge transfer reaction rate across the electrolyte/electrode and electrolyte/interfacial layer interfaces. Bi-layered pellets with tailored nano/micro-rod interfaces has been fabricated (by templated deposition and additive manufacturing) with different rod length to diameter aspect ratios. The EIS data from these cells is de-convoluted and compared with known ionic and electronic transport rates, and charge transfer rates, to create fundamental models of interfacial impedance as a function of 3-dimensional interfacial structure.

Investigate Interfacial Modifications and Cell Performance:

We are investigating two types of materials as interfacial layers in SSLiBs.

For Type 1, we use nonflammable organic electrolytes such as perfluoropolyethers (PFPE) based electrolytes. It has been confirmed that such organic electrolytes cannot catch fire and are intrinsically safe. Although, PFPE-based electrolytes have very low ionic conductivity ($\sim 10^{-5}$ S/cm) and cannot meet the power density requirement in the FOA by itself, PFPE based organic electrolyte can greatly increase the interfaces across electrolyte grain boundaries, or electrolyte/electrode interface for enhancing the battery performance.

For Type 2, we also use a polymer electrolyte or gel electrolyte, which is Bis(trifluoromethane)sulfonimide lithium salt (LiTFSI) in Poly(vinylidene fluoride-co-hexafluoropropylene) (PVDF-HFP). Although the polymer or gel electrolyte has a much lower ionic conductivity, its thickness is small as an interface layer and thus its contribution in overall impedance is negligible. These soft electrolytes can largely improve the contacts between electrodes and electrolytes toward better charge transport and mechanical integrity.

For Type 3, we are investigating thin inorganic layers by atomic layer deposition (ALD) and other thin film deposition techniques to form a nano-thin conducting phase between the garnet and the electrode.

For Type 4, we are using a soft conformable materials such as β -Li₃PS₄ (LPS) or liquids to bridge the gap between the garnet and electrode material.

For each approach, we are fabricating half cells to investigate interfacial impedance and their changes during cycling.

Results and Discussion:

The following progress has been achieved:

Cathode Interface Resistance – Gel Electrolyte Interface:

Gel electrolyte interfacial layers can significantly reduce interfacial impedance between garnet solid state electrolytes and cathodes. Figure 1a is the electrochemical impedance spectroscopy (EIS) plot of a cathode/garnet/cathode symmetric cell without any interfacial layer modification. The total resistance of cathode/garnet/cathode symmetric cell without gel interfacial layer is $\sim 10^6$ Ohm*cm² due to the poor contact between garnet and LiFePO₄ cathode material, the difficulty of charge transfer through the interface between two solid materials, the non-conductive binder, and the rough surface of the garnet pellet.

Figure 1b is the EIS plot of cathode/garnet/cathode symmetric cell with gel interface. The impedance curve has three components. In the high frequency region ($f > 9$ kHz) is an incomplete semi-circle, corresponding to the bulk and grain boundary impedance of the garnet electrolyte. In the middle frequency region ($7 \text{ Hz} < f < 9 \text{ kHz}$) is a combination of two semi-circles corresponding to interfacial charge transfer impedance between garnet and cathode, including impedance on the gel/garnet and cathode/gel interfaces, as the impedance of the gel layer itself is very small. In the low frequency region ($f < 7 \text{ Hz}$) is a straight line, corresponding to diffusion impedance of the cathode.

The interfacial resistance is obtained by subtracting the garnet resistance obtained separately by EIS of garnet samples from the total symmetric cell resistance, then dividing by two as there are two interfaces, e.g.,:

- Thickness of garnet pellet is 500 μ m, and garnet conductivity is 2.1×10^{-4} S/cm (Figure 1c). Therefore, area specific resistance (ASR) of garnet pellet is 239 Ohm*cm².
- The total symmetric cell resistance (Figure 1b) is 600 Ohm*cm². Therefore, the ASR of one interface is $(600-239)/2 = 180$ Ohm*cm², which is ~ 4 orders of magnitude less than the same symmetric cell without the interfacial layers.

To further reduce the garnet/cathode interfacial impedance the procedure was improved by making a gel/cathode composite, instead of using separate gel layers, thus reducing the gel thickness and improving the contact between gel and cathode. Figure 1c shows the structure of symmetric cell using LiFePO₄/gel cathode on both sides of garnet, and Figure 1e shows the impedance of this structure. The corresponding interfacial ASR is now reduced to only 67 Ohm*cm² for one interface (using same approach described above).

Cathode Interface Resistance – Effect of Structure on Interface – 3D Printed Garnet Interface:

A 3D garnet surface structure can dramatically increase the effective surface area relative to the planar areal surface area. 3D structured garnet line patterns were printed on surface polished garnet pellets and sintered to form structured ionic conductive paths with varying line spacing (Figure 2). Cathode slurries (LiFePO₄, CNT, and gel) were coated on both flat and structured garnet surfaces. EIS of the symmetrical cells was obtained at room temperature.

The depressed arcs, which can be assigned to Li⁺ diffusion and charge transfer steps, became much smaller after effective extension of surface area. The 3D printed lines (40 μ m height and 70 μ m width) increased the effective sample surface areas from 36 mm² for polished pellet to 39.9, 42.3 and 48 mm² with increasing line density, resulting in 22%, 35% and 52% reduction of interfacial resistance (from the intercept of real axis high frequency arc (Figure 2a)) proportional to the increase in effective surface area (Figure 2b). Therefore, as expected the 3D printed structures reduced the cathode-electrolyte interfacial resistance linearly with increasing effective surface area. Further impedance reduction is anticipated with increase in line density (using smaller printing tips and reduced particle size).

Cathode Interface Resistance – Aqueous Interface:

To further reduce the cathode/garnet interfacial resistance we evaluated an aqueous solution interface (e.g., Type 4). We anticipated a lower cathode/garnet interfacial resistance with the aqueous interface compared with the gel interface as the aqueous solution has higher conductivity and fluidity than the organic electrolyte used for the gel interfaces. Figure 3a shows a schematic of the symmetric cell with the aqueous cathode/garnet interface. The cathode material (LiFePO₄, Carbon black and PVDF) was coated on a carbon cloth. Then these electrodes were immersed into a saturated aqueous LiCl solution to wet them and then the two electrodes and a garnet pellet were pressed together.

As shown in Figure 3b, the EIS semi-circle of the cell yields a resistance of 253 Ohm*cm², which after correcting for garnet ASR and dividing by 2 for the dual interfaces results in a single

cathode/garnet interfacial resistance of only $7.5 \text{ Ohm}\cdot\text{cm}^2$, 5 orders of magnitude lower than the non-interfacial layer cell, and achieving the Q4FY16 and budget period 2 Go/NoGo milestones.

Li Anode/Garnet Interface – Gel Electrolyte Interface:

Figure 4a shows that the total resistance of a Li/garnet/Li symmetric cell (formed by melting Li metal on the garnet surfaces) without an interfacial layer is about $3000 \text{ Ohm}\cdot\text{cm}^2$. Figure 4b shows the EIS plot of Li/gel/garnet/gel/Li plot has four components. In the high frequency region is an incomplete semi-circle, from the garnet impedance. In the middle frequency region are two semi-circles, due to interfacial charge transfer impedance between garnet and Li metal, which mainly comes from impedance on the gel/garnet and Li/gel interfaces, as the impedance of the gel layer itself is very small. In the low frequency region is a tail, corresponding to diffusion impedance of the interface of gel/stainless steel outside of the lithium metal. Correcting for garnet impedance, the ASR with the gel interlayer is reduced to $200 \text{ Ohm}\cdot\text{cm}^2$ for one interface; however, this is done without melting the Li metal as was done for the other cell.

Li Anode/Garnet Interface – Si Interface:

LLZ and Si-coated LLZ was sandwiched by two Li metal electrodes to assemble symmetric cells (Figure 5a and 5b). Prior to the electrochemical measurements, all the cells were heated at $\sim 200^\circ\text{C}$ for twenty minutes in a glovebox since thermal treatment promotes superior contact between Li and LLZ. Due to the high reactivity of molten Li, lithiated Si will be formed in situ between the Li metal and the Si-coated LLZ. The Nyquist plots of symmetric cells in Figure 5c exhibit two distinct semi-circles: one at high frequency and another at low frequency. The Li/LLZ/Li symmetric cell delivers a large resistance of $2064 \text{ Ohm}\cdot\text{cm}^2$, where the interfacial resistance between Li and LLZ was calculated to be $925 \text{ Ohm}\cdot\text{cm}^2$.

The first semi-circle at relatively high frequency was used to analyze the interfacial resistance between the Li metal electrode and the LLZ solid electrolyte with/without Si coating. As shown in Figure 5d, the overall resistance of the LLZ (bulk and grain boundary) measured using Au electrodes is $215 \text{ Ohm}\cdot\text{cm}^2$. As shown in Figure 5e, the first semi-circle of the Li/LLZ/Li cell yields a resistance of $2064 \text{ }\Omega\cdot\text{cm}^2$, which can be divided into two parts: one is the resistance of the LLZ (bulk and grain boundary) and the other is the Li metal-LLZ interfacial resistance. Thus, the overall Li metal-LLZ interfacial resistance is $1849 \text{ Ohm}\cdot\text{cm}^2$. Since two Li metal-LLZ interfaces are present in the Li/LLZ/Li symmetric cells, the single Li metal-LLZ interfacial resistance is approximately $925 \text{ Ohm}\cdot\text{cm}^2$. On the other hand, the Si-coated LLZ cell displays a much smaller resistance of $469 \text{ Ohm}\cdot\text{cm}^2$ in the first semi-circle. By subtracting the resistance of the LLZ ($215 \text{ Ohm}\cdot\text{cm}^2$) and dividing by two, the Li metal/Si-coated LLZ interfacial resistance can be calculated: $127 \text{ Ohm}\cdot\text{cm}^2$, which is about 7.3 times lower than bare LLZ.

Li Anode/Garnet Interface – Al Interface:

Two symmetric cells, Li | Garnet SSE | Li and Li | Al-Garnet SSE-Al | Li, were prepared and tested directly in an argon-filled glovebox. The two cells showed large differences in total resistance, which depend on both the garnet's total resistance and the interface charge transfer resistance, as shown in the Nyquist plots (Figure 6a and 6b). The Li | Garnet SSE | Li cell had a total resistance of $\sim 2000 \text{ Ohm}\cdot\text{cm}^2$. However, the Li | Al-Garnet SSE-Al | Li cell exhibited a

resistance of $\sim 300 \text{ Ohm}\cdot\text{cm}^2$, which is almost one order of magnitude smaller than the uncoated SSE. The small partial semicircle at high frequency can be assigned to the total resistance of the garnet material. The large semicircle at medium frequency and low frequency correspond to the charge transfer resistance, which is the combination of the solid-state electrolyte resistance as well as the Li interfaces within the symmetric cells. The decreased size of the semicircle indicates that the interfacial resistance was significantly reduced using the Al coating. The total garnet resistance was $\sim 150 \text{ Ohm}\cdot\text{cm}^2$ and remained unchanged during the Li melting process. By subtracting the garnet ASR, the Li | Garnet SSE | Li cell charge transfer resistance was $\sim 1900 \text{ Ohm}\cdot\text{cm}^2$ at 20°C . For the Li | Al-Garnet SSE-Al | Li cell, the charge transfer resistance was decreased to $\sim 150 \text{ Ohm}\cdot\text{cm}^2$. Note that the interfacial resistance corresponds to two symmetric interfaces. Therefore, the interfacial resistance is $\sim 950 \text{ Ohm}\cdot\text{cm}^2$ and $\sim 75 \text{ Ohm}\cdot\text{cm}^2$ for Li | Garnet SSE and Li | Al-Garnet SSE-Al, respectively.

Li Anode/Garnet Interface – ALD Al_2O_3 Interface:

To make Li/garnet/Li symmetric cell with ALD Al_2O_3 interface, a $\sim 5\text{-}6 \text{ nm}$ thick ALD- Al_2O_3 coating was applied to the garnet surface. Then a piece of Li metal foil was pressed on the garnet pellets and heated at 250°C for 1 hour under a small pressure. A control sample was made using bare LLCZN pellets in the same way.

Figure 7a shows the schematic of the interface between garnet and Li metal. The SEM images in Figure 7b clearly demonstrated that the enhancement of interfacial contact by applying ALD Al_2O_3 ultrathin layer on garnet interface. Inset are photo images to show the surface wetting of garnet and the ALD treated garnet.

To quantify the effect of ALD on the improvement of garnet/Li interface, symmetric Li/garnet/Li cells were prepared and evaluated by EIS. As shown in Figure 7c, two distinct arcs were seen in each sample. The bulk garnet ASRs, obtained from the high frequency intercept, are 26 and $28 \text{ Ohm}\cdot\text{cm}^2$ for cells with and without ALD coating, respectively. The first arc represents most likely the grain boundary impedance which were $150 \text{ Ohm}\cdot\text{cm}^2$ and $4500 \text{ Ohm}\cdot\text{cm}^2$ for cells with and without ALD coating, respectively. The second lower frequency arc is characteristic of the interfacial impedance. Interfacial ASR was calculated by dividing this resistance by two before normalizing to the electrode surface area. It can be seen that the ALD treatment decreased the interfacial ASR by EIS from $490 \text{ Ohm}\cdot\text{cm}^2$ to $16 \text{ Ohm}\cdot\text{cm}^2$.

The cells were also tested under DC cycling. As shown in Figure 7d the symmetric cell with bare garnet had an unstable voltage profile with large voltage over-potential with peak voltage values over 4 volts. In contrast, for the symmetric cell with ALD treated garnet, the stable voltage profile with small voltage range demonstrates that the interfacial resistance between garnet and Li metal was effectively reduced. Inset gives a single cycle of the symmetric ALD treated garnet cell to show the small and flat voltage plateau ($\sim 15 \text{ mV}$). From this comparison, the Li/garnet/Li symmetric cell without ALD has an unstable DC resistance, over 260 times ($4\text{V}/15\text{mV}$) larger than the DC resistance of the cell treated with ALD. Figure 7e presents the long-term cycling performance of the symmetric ALD treated garnet cell at a current density of $0.2 \text{ mA}/\text{cm}^2$. The cell voltage increased slightly from 15 mV to 20 mV after 30 hours and remained stable for 130 hrs. This cell voltage (20 mV) corresponds to a total cell ASR of $100 \Omega\cdot\text{cm}^2$ which is the sum of the total electrolyte ASR and both interfaces.

Modeling of Interfacial Coating Layers on Garnet-Electrode Interfaces:

We applied first principles calculations to investigate the interface stability between garnet and formed Li-Al alloys. We considered the interface as a pseudo-binary of Li-Al alloy and garnet, then constructed the related phase diagram to identify possible thermodynamically favorable reactions. The compositional phase diagrams were constructed, and the mutual reaction energy of the pseudo-binary calculated using same approach defined in our previous work. We found that three kinds of Li-Al alloy showed mutual reactions with garnet because of the slightly thermodynamic “welding” at their interface. Since the calculated reaction enthalpy is only around $-60 \sim -40$ meV/atom, the small reaction energy indicates that the interfacial reactions are likely to be limited and the formed interface could be relatively thermodynamic stable. Therefore, the interface between Li-Al alloy and garnet may exhibit good chemical stability, which might facilitate Li ion transport through.

We apply the computational scheme to investigate interfacial chemical compatibility of these two interfaces with the coating layer with the SE and LCO, respectively. The previously demonstrated coating layer materials, such as $\text{Li}_4\text{Ti}_5\text{O}_{12}$, LiTaO_3 , LiNbO_3 , Li_2SiO_3 , and Li_3PO_4 , have excellent chemical stability with the LCO and $\text{L}_{0.5}\text{CO}$ with zero or negligible decomposition energy $\Delta E_{\text{D,min,mutual}}$ (Table 2). In addition, all coating layer materials show relatively better stability with the sulfide SE comparing to the original sulfide SE-LCO interfaces, which have the interfacial reaction energy $\Delta E_{\text{D,min,mutual}}$ of ~ -500 meV/atom. As a result, the interface with the coating layer has significantly improved stability and suppresses the formation of thick interphase layer. In addition to stabilizing the interface, the coating layer of only a few nanometers is significantly thinner than the decomposition interphase layer of ~ 10 to 100 nm. The reduced thickness of the coating layer may significantly reduce the high interfacial resistance caused by the thick decomposition interphase layer.

In addition, we also computationally investigated other compounds (listed in Fig. 9 and Table 2) based on the same cations, such as Ti, Nb, Si, Ta, and P, as potential coating layer materials. All these lithium metal oxide materials have a wide electrochemical window (Fig. 9a). The compounds with higher Li content generally show lower reduction potential, and the compounds with lower Li content or higher O content show higher oxidation potential. Most of these compounds have excellent chemical stability against LCO and $\text{L}_{0.5}\text{CO}$ cathode materials with zero or small $\Delta E_{\text{D,min,mutual}}$ (Table 2). All these coating layer materials significantly improve the stability of sulfide SE-LCO interfaces. The chemical stability between LLZO-coating layer interface varies significantly with the compositions of the coating layer materials. The other Li-rich coating layers, such as Li_4TiO_4 , Li_2TiO_3 , Li_8SiO_6 , Li_4SiO_4 , Li_5TaO_5 , and Li_3TaO_4 may work better with LLZO than those previously demonstrated for sulfide SEs, such as $\text{Li}_4\text{Ti}_5\text{O}_{12}$, LiTaO_3 , and Li_2SiO_3 .

Conclusions:Garnet-Cathode Interface:

- We demonstrated that gel electrolyte can reduce the interfacial resistance by over 4 orders of magnitude achieving an interfacial ASR of ~ 67 $\text{Ohm}\cdot\text{cm}^2$ for planar cathode/garnet interface.

- We demonstrated that increasing surface area can effectively decrease the interface resistance, achieving a 52% decrease in interfacial ASR so far. Further increasing the surface area with 3D printing we expect we can decrease the above gel interface resistance with a planar structure by another 10X achieving an interfacial ASR of $\sim 7 \text{ Ohm}\cdot\text{cm}^2$.
- However, the aqueous interface lead to $7.5 \text{ Ohm}\cdot\text{cm}^2$ cathode/garnet interfacial resistance planar cathode/garnet interface. Therefore, we have met the $\sim 10 \text{ Ohm}\cdot\text{cm}^2$ garnet/cathode milestone without need of modifying interface 3D structure.

Li-Garnet Interface:

- We demonstrated gel electrolyte, Si, and Al can reduce interfacial resistance to $200 \text{ Ohm}\cdot\text{cm}^2$, $127 \text{ Ohm}\cdot\text{cm}^2$, and $75 \text{ Ohm}\cdot\text{cm}^2$, respectively for planar Li metal-garnet interface.
- We further demonstrated that ALD- Al_2O_3 can reduce interfacial resistance to $16 \text{ Ohm}\cdot\text{cm}^2$ for planar Li metal-garnet interface. Therefore, we have met the $\sim 10 \text{ Ohm}\cdot\text{cm}^2$ garnet/anode milestone.
- Similar to what was demonstrated with the cathode/electrolyte structure effect, we expect a 52% reduction (the same as the cathode) by using 3D printed garnet, as demonstrated in the report, this would corresponds to only $\sim 8 \text{ Ohm}\cdot\text{cm}^2$ anode/garnet ASR. Moreover, increasing the surface area with 3D printing we expect we can decrease the above ALD interface resistance with a planar structure by another 10X.

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Figures and Tables:

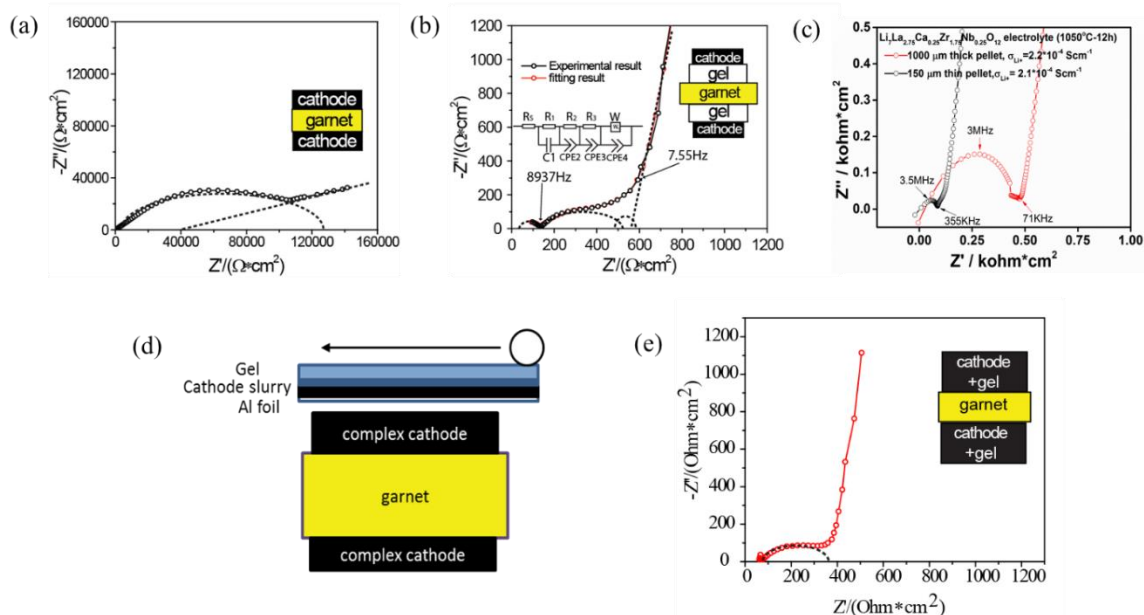


Figure 1. (a) EIS plot of cathode/garnet/cathode symmetric cell without gel electrolyte. (b) EIS of cathode/gel/garnet/gel/cathode symmetric cell and the equivalent circuit. (c) EIS of garnet itself. (d) Schematic of making garnet cell with mixed cathode. (e) EIS figure of symmetric cell with mixed cathode and gel.

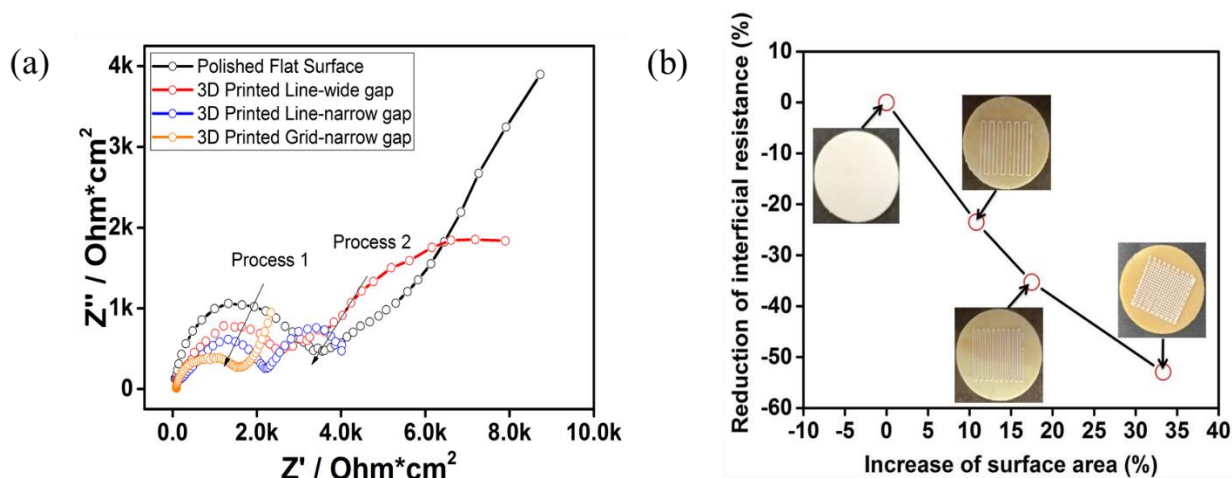


Figure 2. Comparison of cathode/electrolyte interfacial impedance on flat and 3D-structured garnet pellets. (a) EIS plot of garnet without 3D printing and with different 3D printings. (b) Reduction of interfacial resistance with increase in surface area.

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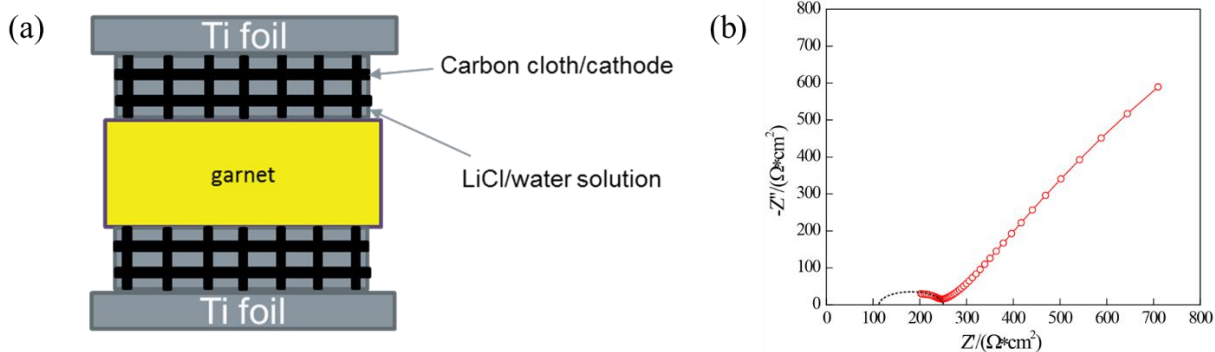


Figure 3. (a) Schematic of a cathode/garnet/cathode symmetric cell with aqueous interface. (b) Impedance of this cell with aqueous interface.

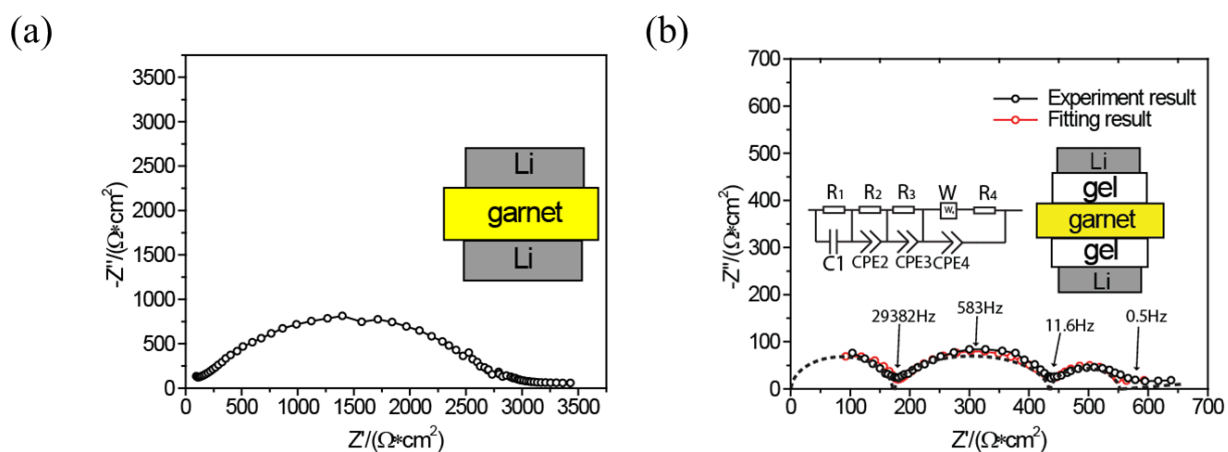


Figure 4. (a) EIS plot of Li/garnet/Li symmetric cell. (b) EIS plot and equivalent circuit of Li/gel/garnet/gel/Li symmetric cell.

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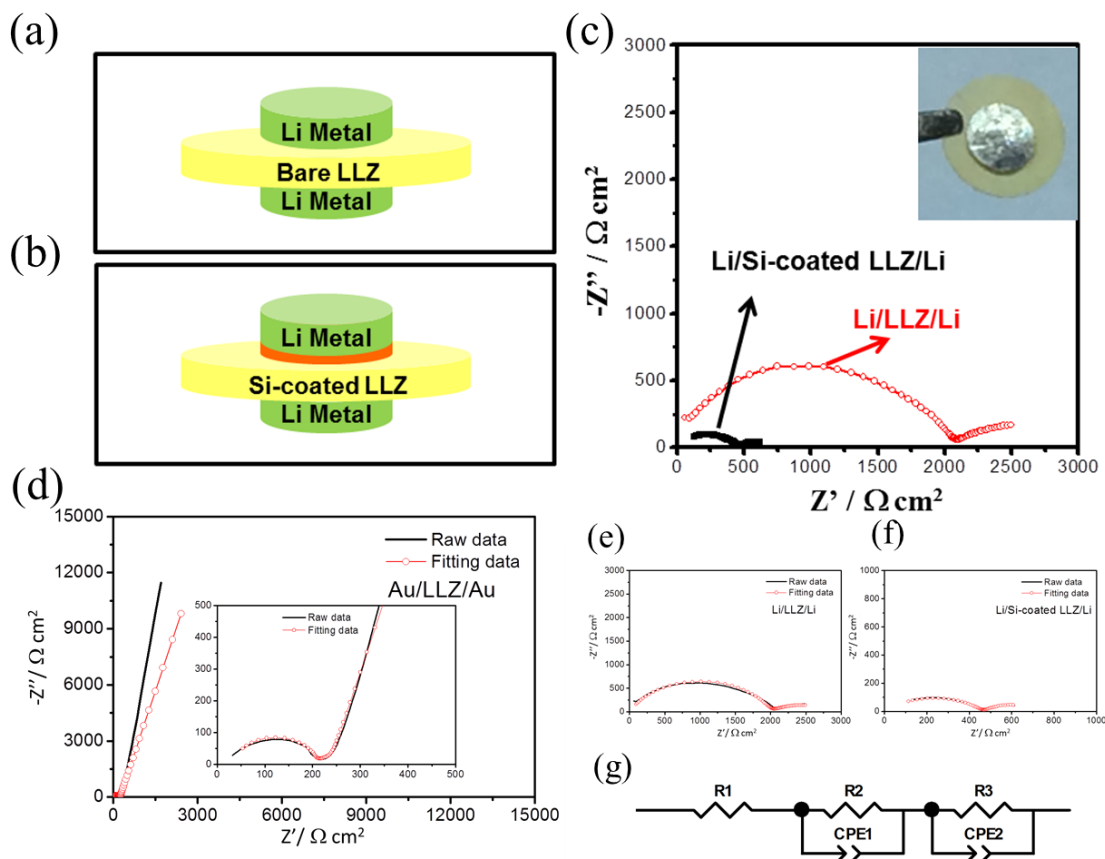


Figure 5. Schematic illustration showing the structure of symmetric cells with (a) LLZ or (b) Si-coated LLZ SSEs. (c) Electrochemical impedance spectroscopy (EIS) measurements of symmetric cells where the interfacial resistance of the Si-coated garnet cell significantly decreased. Inset of (c) is a digital image of a Li/Si-coated LLZ/Li symmetric cell. (d) Nyquist plots of the Au/LLZ/Au symmetric blocking electrode system at room temperature. The solid black line denotes the experimental data while the red line with hollow spheres represents the fitting data using the equivalent circuit modeling. (e-g) Nyquist plots of (e) Li/LLZ/Li and (f) Li/Si-coated LLZ/Li symmetric cells. (g) The equivalent circuit model used in this study.

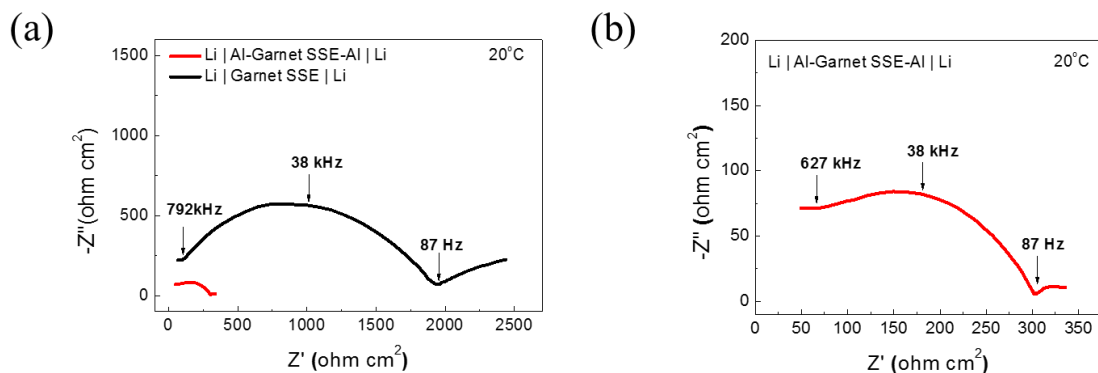


Figure 6. Nyquist plots of Li | Garnet SSE | Li (a) and Li | Al-Garnet SSE-Al | Li (b) in the frequency of 1 MHz to 100 mHz at 20°C.

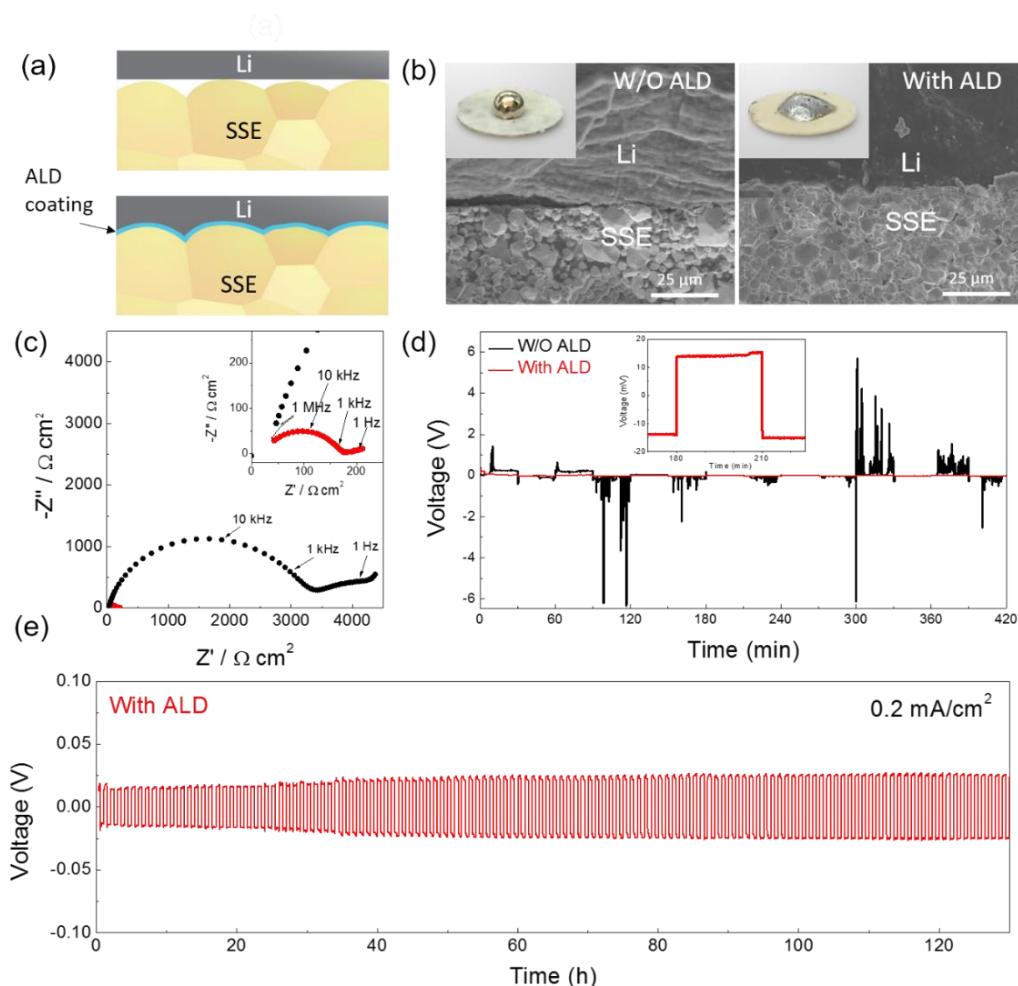


Figure 7. Characterization of garnet solid state electrolyte/Li metal interface. (a) Schematic of the wetting behavior of garnet surface with molten Li. (b) SEM images of the garnet solid state electrolyte/Li metal interface. Without ALD Al_2O_3 coating, garnet has a poor interfacial contact with Li metal. Inset are photo images of contacts between melted Li metal and garnet surface. (c) Comparison of EIS profiles of the symmetric Li non-blocking garnet cells. Inset shows the enlarged impedance curve of the ALD treated garnet cell. (d) Comparison of Li tripping/plating behavior of the symmetric garnet SSE/Li cells. Inset is the one cycle of stripping/plating for the ALD treated garnet cell, exhibiting a low overall impedance and stable interfacial property. (e) Voltage profile of the ALD treated garnet symmetric cell at a current density of 0.2 mA/cm^2 .

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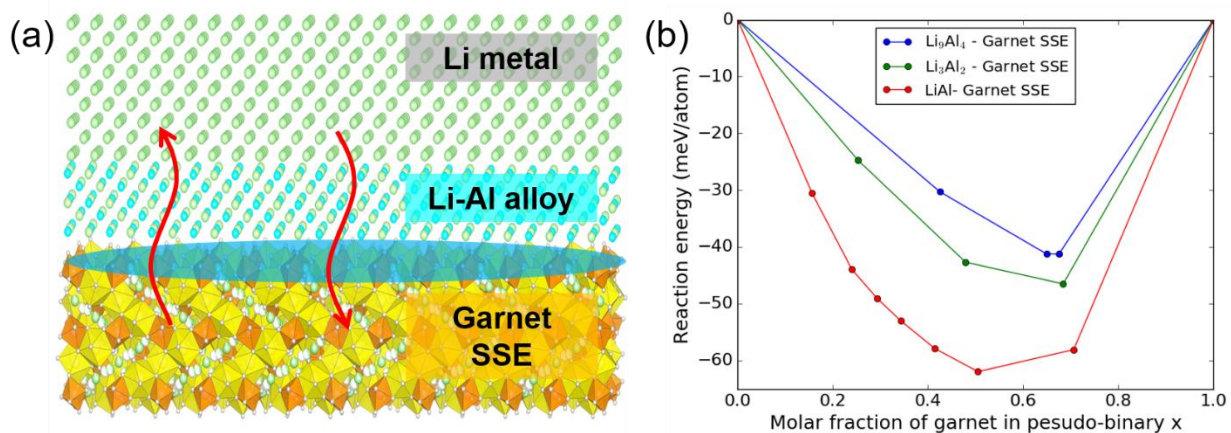


Figure 8. Calculated mutual reaction energy, ΔE_D , of garnet and Li-Al alloy interfaces.

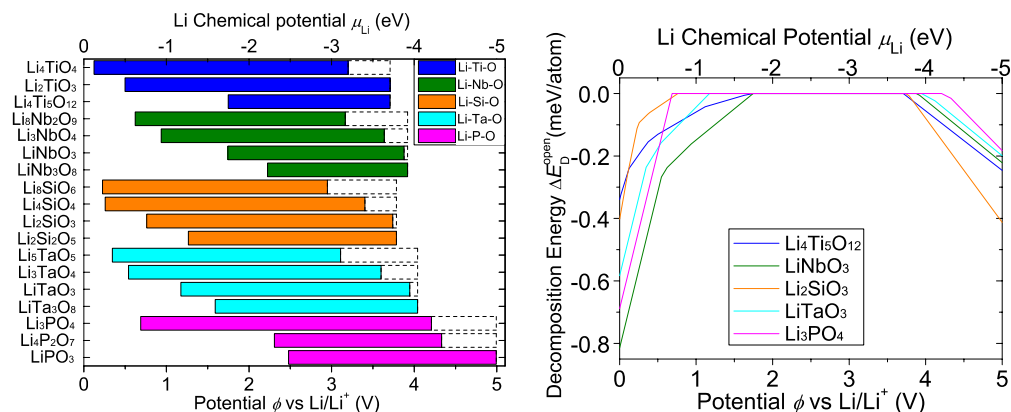


Figure 9. Electrochemical window (left) and the decomposition energy ΔE_D^{open} (right) of the proposed and previously demonstrated coating layer materials applied between SE and cathode materials.

The dashed line in (a) marks the equilibrium voltage to fully delithiate the materials.

LLCZN	Bulk	Grain	Grain	Interfacial	Interfacial
SSE	ASR	boundary	boundary	ASR	capacitance
	($\Omega \cdot \text{cm}^2$)	ASR	capacitance	($\Omega \cdot \text{cm}^2$)	(F)
		($\Omega \cdot \text{cm}^2$)	(F)		
No ALD	28	4500	2.09×10^{-9}	490	9.9×10^{-4}
ALD	26	150	3.09×10^{-9}	16	2.8×10^{-5}

Table 1. Electrochemical impedance ASR with fitting data for Li/LLCZN/Li cells with and without ALD coating on both sides of garnet SSEs.

	Li ₃ PS ₄	LLZO	LCO	L _{0.5} C O
Li ₄ TiO ₄	-125	0	0	-30
Li ₂ TiO ₃	-75	-5	0	0
Li ₄ Ti ₅ O ₁₂	-80	-75	-1	0
Li ₈ Nb ₂ O ₉	-147	0	0	-20
Li ₃ NbO ₄	-132	-4	0	0
LiNbO ₃	-155	-76	0	0
LiNb ₃ O ₈	-173	-115	-16	0
Li ₈ SiO ₆	-177	0	-3	-50
Li ₄ SiO ₄	-81	-1	0	-12
Li ₂ SiO ₃	-19	-29	0	0
Li ₂ Si ₂ O ₅	-10	-69	-4	0
Li ₅ TaO ₅	-117	0	0	-32
Li ₃ TaO ₄	-64	-3	0	0
LiTaO ₃	-49	-68	0	0
LiTa ₃ O ₈	-64	-105	-22	0
Li ₃ PO ₄	0	0	0	0
Li ₄ P ₂ O ₇	-9	-101	-44	-3
LiPO ₃	-32	-201	-76	-19

Table 2. The mutual reaction energy $\Delta E_{D,min,muual}$ (in meV/atom) of the coating layer materials with the SE or LCO materials.

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AVPTA Technology Focus Area 6: Energy Storage & Batteries

Beyond Li-Ion: New Lamination and Doping Concepts for Enhanced Li-Sulfur Battery Performance

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Project Start: Q2FY14
Estimated Completion: Q4FY17

Objective:

- To successfully demonstrate generation of novel sulfur cathodes for Li-S batteries meeting the targeted gravimetric energy densities ≥ 350 Wh/kg and ≥ 750 Wh/l with a cost target \$125/kWh and cycle life of at least 1000 cycles for meeting the EV everywhere blueprint. The proposed approach will yield sulfur cathodes with specific capacity ≥ 1400 mAh/g, at ≥ 2.2 V generating ~ 460 Wh/kg, energy density higher than the target. Full cells meeting the required deliverables will also be made.

Strategic Context:

- Generate a leap-ahead technology used for military vehicles to support the future power for TARDEC and the Army by enabling the development of advanced battery systems with significant increases in energy density
- Improve Battery safety characteristics to support vehicle silent watch and enable other high energy requiring applications.

Accomplishments:

- Demonstrated capabilities for generation of novel sulfur 1-D, 2-D and 3-D morphologies exhibiting superior stability and capacity (June 2015)
- Identified and synthesized LIC materials for use as coatings for sulfur cathodes (June 2015)

- Identified suitable dopants and dopant compositions to improve electronic conductivity of sulfur (October 2015)
- Demonstrated synthesis of doped LIC membrane with improved Lithium-ion conductivity (December 2015)
- Identified and developed effective coating methods to form a uniform lamina of LIC membrane over sulfur hetero-structures (March 2016)
- Identified suitable dopants and dopant compositions to improve electronic conductivity of sulfur (October 2015)
- Conducted fundamental electrochemical study to understand the reaction kinetics, mechanism and charge transfer kinetics (October 2015)
- Prepared doped LIC with improved ionic conductivity (January 2016)
- Demonstrated synthesis of doped LIC membrane with improved Lithium-ion conductivity (January 2016)
- Developed CFN morphology with a stable cycling performance of ~650 mAh/g for over 300 cycles with < 0.02% fade rate (April 2016)
- Accomplished demonstration of binding of polysulfide with CFN results in polysulfide retention and hence, improved cycling stability (April 2016)
- Demonstrated the effect of the unique pore size (~2nm) of CFN preventing dissolution of polysulfide from the liquid electrolyte (April 2016)
- Demonstrated stable capacity of ~550 mAh/g over 100 cycles with the application of TPM improved the specific capacity of commercial sulfur (April 2016).
- Developed novel lithium-ion conducting (LIC) membrane systems using *ab-initio* methods displaying impermeability to sulfur diffusion (December 2014)
- Demonstrated capabilities for generation of novel sulfur 1-D, 2-D and 3-D morphologies exhibiting superior stability and capacity (June 2015)
- Identified suitable dopants and dopant compositions to improve electronic conductivity of sulfur (October 2015)
- Performed fundamental electrochemical study to understand the reaction kinetics, mechanism and charge transfer kinetics (October 2015)
- Prepared doped LIC with improved ionic conductivity (January 2016)
- Conducted study on doping Sulfur with dopants of similar size to sulfur with enhanced electronic properties (April 2016)
- Completed developing organic and inorganic Complex Framework materials (CFM) as effective polysulfide traps (July 2016)
- Started synthesis of VACNT and LIC coated nanosulfur based composite materials (January 2017) – Ongoing
- Continue to design and engineering of high capacity LIC coated sulfur nanoparticle (January 2017) – Ongoing

Introduction:

The increasing demand in the EV industry for low cost, light weight and high energy storage batteries to meet the EV everywhere grand challenge, the current focus of research has

shifted towards the development of lithium sulfur (Li-S) batteries owing to the high theoretical specific capacity exhibited by sulfur compared to other cathode materials currently available. Li-S battery shows a theoretical capacity of 1675 mAh/g corresponding to the formation of Li_2S which makes sulfur a promising electrode to replace the layered transition metal oxides (~ 150 mAh/g) and LiFePO_4 (~ 170 mAh/g) deployed in present LIB systems. Moreover, the abundance of sulfur in the earth's crust, its ubiquitous availability as a byproduct in the extractive mineral and petrochemical industry, combined with ease of processing, makes it a more economical proposition compared to currently existing cathode materials.

Approach:

The objectives outlined above will be accomplished by engineering sulfur cathode materials primarily by laminating the electrodes with lithium ion conductor (LIC) coatings in order to prevent polysulfide dissolution and doping in order to improve the electronic and ionic conductivity. The following major technology innovations will be undertaken to accomplish the following objectives of this effort:

- Phase – 1 (Year 1): Synthesis, Characterization and Scale up of suitable LIC matrix materials and multilayer composite sulfur cathodes. This phase is completed.
- Phase – 2 (Year 2): Development of LIC coated sulfur nanoparticles, scale up of high capacity engineered LIC coated multilayer composite electrodes and doping strategies for improving the electronic conductivity of sulfur.
 - Optimize and scale up of interface engineered multilayer composite LIC coated sulfur cathode architectures exhibiting: Specific capacity ≥ 1200 mAh/g (≥ 4 mAh/cm²), cyclability (~ 1000 cycles), loss per cycle: $\leq 0.01\%$ per cycle, CE: $\geq 80\%$.
 - Synthesize and scale up of doped sulfur nanoparticles on gram scale and demonstrate improvement in performance, reflected as an increase in sulfur weight percentage and improvement in rate capability of cycling of the electrodes.
- Phase-3 (Year 3): Advanced high energy density, high rate, and highly cyclable cell development.
 - Tie together the three different trees of development i.e. coating development/sulfur particle development/CNT based exploration by identifying suitable configuration integrated electrode (I.E.) with maximum sulfur weight percentage demonstrating high capacity ≥ 1400 mAh/g, cyclability (~ 1000 cycles), loss per cycle: $\leq 0.01\%$ per cycle, CE: $\geq 80\%$.
 - Assemble 4 mAh high energy density Li-S pouch cells and performance testing.

Results and Discussion:

Phase-1 of the current project concluded with the successful identification of effective lithium-ion conducting (LIC) membrane and demonstration of the ability of LIC to shield the polysulfide species from dissolving into the electrolyte. To achieve this target, 4 strategies outlined in the following were employed during *Phase-1* of the project: (a) Use of inorganic LICs in the form of pellet coatings (Q1, Q2) (b) fabrication of flexible polymer-sulfur wires (Q2) (c) generation of gel polymer electrolyte (GPE) as an electrolyte medium (Q3) (d) use of complex framework materials (CFM) as trapping agents for sulfur species (Q4). These strategies resulted in improved cycling with scope for further improvement. The aim of *Phase-2* studies is to

synthesize novel doped LIC materials with high lithium ion conductivity identified in *Phase 1*, to develop effective coating strategies of these materials and to generate hetero structured composites of sulfur with carbon materials. Towards this end, the following strategies were employed during *Phase-2* of the project: (a) Improving ionic conductivity of lithium ion conductors using first-principles driven doping approaches (b) Composite polymer electrolytes demonstrating no capacity loss in commercial sulfur electrodes (c) Sulfur infiltrated framework (SFM) materials with chemical trapping of sulfur (d) Altering the electronic structure of sulfur with size matched dopants. The results of these studies follow.

Improving Ionic Conductivity of Lithium-Ion Conductors using First-Principles-Driven Doping Approaches:

In FY14, it was demonstrated using density functional theory (DFT) studies that an improvement in ionic conductivity can be achieved upon the introduction of vacancies in the lattice of Li ion conductor Li_4SiO_4 . Li_4SiO_4 is a very wide band gap insulator with strong Si-O hybridization, covalent Si-O bonds and ionic Li-O, large channels for Li-conduction with Li^+ ionic conductivity ($\sim 10^{-12}$ S/cm). The effect of doping (dopants- D_1 and D_2) on Li sites and F doping on O sites of Li_4SiO_4 on its ionic conductivity was investigated using first principles calculations in Phase-1. Nudged elastic band method has been used for determining the potential energies and activation barriers E_a for various Li-ion migration pathways in pure and doped Li_4SiO_4 . These calculations suggest a decrease in the activation barrier (Figure V - 1) for Li^+ ion conductivity because of doping. The unit cell of Li_4SiO_4 contains two SiO_4^{-4} tetrahedra linked by 8 lithium ions, which are distributed over 18 possible sites. At room temperature, an improvement in ionic conductivity of 3 to 4 orders in magnitude could be obtained by forming simple solid solutions.

To validate the theoretical predictions, cation and anion doping of Li_4SiO_4 was performed to obtain final materials of the chemical formula shown by i and ii.

- i. $(\text{Li}_y[\]_x\text{Y}_x)_4\text{SiO}_4$, where Y – D_1 , D_2 , [] – vacancy, x – 0.025 to 0.15
- ii. $\text{Li}_4\text{Si}(\text{O}_y[\]_x\text{Z})_4$, where Z – D_3 , [] – vacancy, x – 0.025 to 0.15

Solid state high temperature processing route from suitable precursors was employed to generate doped nanoparticles of LIC. Different precursor ratios were used to tailor the atomic % of lithium vacancies in the LIC and tested for ionic conductivity. Lithium orthosilicate was doped with six different concentrations (2.5 at. %-15 at. %) of each dopant using a high temperature solid state diffusion technique. The X-ray diffraction (XRD) patterns of the various compositions of doped lithium orthosilicate indicate that a maximum of 7.5% lithium sites was successfully doped with the two different cations (D_1 and D_2). Further increase in the dopant concentration results in formation of secondary phases. Similarly, up to 7.5% oxygen sites were replaced with dopant D_3 maintaining phase purity, with secondary phases appearing upon excessive D_3 doping. Figures V – 2 (a-c) show the results of electrochemical impedance spectroscopy (EIS) analysis of the doped lithium orthosilicate materials and Figure V - 2d depicts the ionic conductivity dependence on dopant concentration in the various doped materials. Creation of vacancies in the LIC crystal structure by doping with D_1 (~ 7.5 at. %) resulted in an increase in ionic conductivity from 1.179×10^{-12} S cm^{-1} to 2.870×10^{-8} S cm^{-1} as seen in Figure V - 2d. Doping with D_2 (7.5at. %) and D_3 (10 at. %) results in a 3-order improvement in the ionic conductivity occurring close to the highest doped concentration (Table V - 1). A comprehensive study utilizing sputter deposition technique to form uniform ultrathin coatings of LIC onto sulfur heterostructures

is ongoing. These doped materials are currently being tested as LIC coatings in nano-sulfur based materials.

Composite Polymer Electrolytes (CPE) Demonstrating No Capacity Loss in Commercial Sulfur Electrodes:

Work in *Phase-1* of this project involved generation on lithium ion conducting polymeric membranes (LICMs) i.e. gel polymer electrolytes (GPEs) for use as separators in lithium-sulfur batteries. These polymeric LICM materials were used in place of conventional polymeric separator materials and it is expected that they will exhibit superior mechanical properties, flame-resistance and flexibility. To tackle capacity fade associated with the conventional gel-polymer electrolyte materials without fillers, nanoparticulate solid state materials were used as fillers in the GPE matrix. Stability improvement because of using doped solid-state nanoparticles as filler materials in the polymer material resulted in a stable capacity of ~400 mAh/g seen up to 80 cycles. The LICMs with solid state systems acting as tethering sites serve as filters to restrain the polysulfide ensuring improvement in cycling stability. Continuing optimization work into the same undertaken as a part of *Phase-2* included engineering of the nature of the LICM materials with regards to polymer composition, filler material composition, particle size and porosity.

As a subtask of Q2, a free standing solid state systems incorporated polymer membrane (SSPM) was used as a sieve to restrain the polysulfides from reaching the anode. The SSPM was used in addition to commercial separator to test with commercial sulfur cathode. Incorporation of the SSPM improved the specific capacity of commercial sulfur to ~550 mAh/g for over 100 cycles. This improvement in specific capacity arises from the binding of the polysulfide species onto the solid state functional moieties. Q4 of *Phase-2* involved the development of composite polymer electrolytes (CPE) with solid-state fillers using simple wet-chemical techniques that demonstrated high capacity and prevention of polysulfide dissolution. The CPE demonstrated an electrolyte uptake of ~200 wt% (Figures V - 3a) with room temperature ionic conductivities (Table V – 2) similar to organic liquid electrolytes. In addition, it can be seen in Figures V - 3b and Figures V - 3c that the CPE materials possess significantly better mechanical properties (Table V – 3) and flame-resistance as compared to commercial separators making them ideal candidates for use in a lithium anode based system on account of improved safety. Testing of these CPEs with commercial sulfur cathodes showed an initial capacity of ~894 mAh/g which remained very stable demonstrating capacity of ~809 mAh/g after 50 cycles (Figure V - 2d). Commercial sulfur electrodes normally undergo capacity loss to <100 mAh/g after 10 cycles. Thus, the CPE material demonstrates significant advancement in sulfur electrolytes. The cycling stability of the cathodes tested with CPE is likely due to the physical properties and optimized electrolyte content of these separator – electrolytes.

Altering the Electronic Structure of Sulfur with Size-Matched Dopants:

Another essential challenge this work aims to undertake is to increase the overall electrode capacity in sulfur cathodes by increasing the inherent electronic conductivity of sulfur. Towards this end, first principles studies were performed in *Phase-1* of the study and suitable doping elements were identified to modify the electronic properties of sulfur resulting in its transformation from an insulator material to a semi-conductor/metallic conductor. Q3 of *Phase-2* also involved successfully doping commercially obtained sulfur (S_8) with similar sized dopants (Figure V – 4) shows the XRD patterns of doped S) to alter the electronic structure and enhance

the electronic conductivity of S. A comprehensive study of the effect of doping of sulfur on rate capability is ongoing.

Sulfur-Infiltrated Framework (SFM) Materials with Chemical Trapping of Sulfur:

A final portion of the study in *Phase-2* involved use of framework to host sulfur and entrap polysulfides during cycling, and ensure capacity retention. The strategy with such host-based framework is two-pronged as follows: (a) the host acts as a conductive matrix; and (b) polysulfide species formed during lithiation are trapped inside the host matrix. Work in *Phase-1* had identified complex framework materials (CFM) with sulfur infiltrated into the nanopores demonstrating very stable cycling with fade rates $<0.01\%$ loss per cycle after a short initial capacity fade. Despite improvements in stability, these structures exhibit an initial capacity loss, the origin of which was explored using X-ray photoelectron spectroscopy studies. Two variants of sulfur infiltrated CFMs, CFM-1 and CFM-2 were synthesized at room temperature and infiltrated with sulfur. The CFMs were used as cathodes for Li – S batteries. CFM-1 shows a very high initial capacity of 1476 mAh g^{-1} , which is the highest capacity value reported in the literature to date¹⁻³, stabilizing at 609 mAh g^{-1} over 200 cycles. The almost negligible fade rate (0.0014% loss cycle⁻¹) and complete prevention of polysulfide dissolution makes these cathode systems most promising candidates for Li-S batteries. However, there is an initial loss in capacity observed and to address this initial capacity loss observed in this system, the mechanism of lithiation and any other side reaction (e.g. SEI formation) involved in the electrochemical lithiation process needs to be understood. To rationally design sulfur hosts using complex framework materials (CFM), a basic understanding of the mechanisms involved in trapping polysulfide into the host materials needs to be established. This mechanism would further explain the origin of irreversible capacity loss during the initial cycles. The work uses XPS analysis as a technique to understand the mechanism involved in masking polysulfide dissolution by directly binding the sulfide species onto the CFMs. The proposed concept of using chemical bonding has been reported elsewhere although complete prevention of polysulfide dissolution and retention has not been reported in the open literature to date⁴. The XPS technique was accordingly used to study polysulfide dissolution and to understand S – CFM bonding providing insight into prevention of the polysulfide dissolution in the current work. The mechanistic overview provided by this report could in our opinion lay the foundations and further identify possible pathways for implementing future design strategies to enhance the capacity and directly aim to resolve polysulfide dissolution problems in the initial cycles plaguing the Li-S battery cathodes.

Table V – 4 represents the BET specific surface area and average pore sizes of both the CFM materials. Both materials exhibit a very high surface area of $\sim 526 \text{ m}^2 \text{ g}^{-1}$, and $\sim 684.25 \text{ m}^2 \text{ g}^{-1}$, respectively with an average pore size of $\sim 2.47 \text{ nm}$. The CFMs were found to have high pore volume of $\sim 0.324 \text{ cm}^3 \text{ g}^{-1}$ and $\sim 0.422 \text{ cm}^3 \text{ g}^{-1}$. To prove the nanoporous nature of CFMs and the binding of sulfur to CFM, TEM analysis was employed (Figure V - 5). It is noteworthy that these surface areas are greater than those of most carbonaceous host materials that have reportedly been used as sulfur hosts in Li – S batteries⁵⁻⁸. The large pore volume of the CFM materials is expected to facilitate in ensuring larger amounts of sulfur encapsulation and thus high sulfur loading in the electrodes. Another unique advantage yielded using CFM materials to encapsulate sulfur is the small average pore diameter of the CFMs (2.46 nm) that aids in minimizing polysulfide dissolution by offering a better mode for trapping and confining the polysulfide species.

The TEM images of CFM-1 at a lower magnification (Figure V - 5a) shows the highly porous nature of the CFM. Phase contrast image of S infiltrated CFM-1 (Figure V - 5b) clearly shows ~5nm islands of sulfur inside the parent CFM structure indicating sulfur infiltration into the CFM. Figure V -5c demonstrates the local-ordering in the CFM structure. The nature of sulfur inside the CFM structure can be seen in Figure V - 5d wherein clear lattice fringes corresponding to sulfur infiltrated within the CFM structure are observed. Two different values of d – spacing, 0.201 nm and 0.277 nm were identified by analyzing the inter-planar distance in the fringes seen in Figure V - 5d.

The nature of sulfur in the S – CFMs was studied using XPS analysis (Figure V - 6). XPS analysis was performed on a Thermo ESCALAB 250Xi with suitable background correction. It can be observed that the characteristic $S2p_{3/2}$ peak is observed for the commercial sulfur powder at 165.21 eV in line with previous reports for orthorhombic sulfur (S_8)⁹⁻¹². The XPS spectra of S-CFMs show a shift in the $S2p$ peak as compared to commercial sulfur indicating the absence of free elemental sulfur suggesting binding of sulfur to the CFM structures. The $S2p_{3/2}$ peak position at 162.45 eV corresponding to the binding of sulfur onto the CFMs is similar to values observed in chemically-bound sulfur studied by Chehimi et al.,¹³ further confirming the bound nature of sulfur onto the CFMs. This chemical binding of sulfur along with the nanoporous nature of the CFMs is expected to result in minimal sulfur dissolution into the organic liquid electrolyte¹⁴. This effect has been observed in sulfur entrapped in single wall carbon nanotubes (SWCNTs) of ~1.5nm diameter by Fujimori et al.¹⁰ wherein sulfur adopts either a linear or a zig-zag orientation as opposed to the conventional cyclic S_8 rings of S. Due to an average pore size of 2 nm of CFMs, comparable to the SWCNTs (~2 nm) used, the sulfur strands might experience strain from the CFM pore walls thus yielding a lower $S2p$ binding energy. The complete trapping of the polysulfide in a host matrix however, has not been reported in the literature and it is expected that further optimization of the CFM materials using a mechanistic understanding gained from the rest of this study would help engineer very high capacity cathodes with almost no capacity fade.

Though both CFM materials exhibit excellent cycling stability after initial stabilization, a significant portion of the initial observed capacity is lost within the 1st ten cycles. This loss is typically attributed to the dissolution of sulfur into the electrolyte and loss of the eventual polysulfide species. However, the stabilization of the capacity following the initial loss appears to draw credence to the possibility of the confinement occurring but the alluding to the possible existence or evidence of other extraneous sacrificial reactions. This result thus implied that the origin of the initial capacity loss in these S – CFMs needs to be better understood warranting better characterization to be conducted to be able to improve the overall performance of the CFM based sulfur electrode system.

The effect of sulfur encapsulation within the CFM structures on the cycling performance of S – CFMs was studied by analyzing the separators retrieved using XPS after 200 charge – discharge cycles. $S2p$ peaks were analyzed to understand the nature of the sulfur/polysulfide species present in the various separators. As control experiments, the commercial separator and commercial separator dipped in the lithium electrolyte were also analyzed and the resultant XPS plots are shown in Figure V - 7 (a, b). As expected, the Celgard separator does not display an $S2p$ peak before cycling while a distinct peak corresponding to the electrolyte species (Trifluoro methyl sulfonate lithium salt) is seen in Figure V – 6b¹⁵. The XPS plot for the post-

cycled separator for the commercial sulfur electrode shows S2p peaks at 168.35 eV, 166.02 eV and 161.45 eV. The peak at 168.35 eV corresponds to S2p peak of cyclic S₇, S₈. On the other hand, the peaks at 166.02 eV and 161.45 eV are due to lower and higher order polysulfide, respectively.¹⁶⁻¹⁹ This indicates and validates the well-known phenomenon of the commercial sulfur electrode (Figure V – 6) undergoing rapid loss in capacity due to the rapid dissolution of polysulfide species formed because a lack of any medium or mechanism to retain/constrict the same at the electrode surface. However, the separators corresponding to the S – CFM electrodes (post-cycling, after 200 cycles) (Figure V – 6 (d, e)) distinctly display only a single S2p peak at 169 eV which corresponds to the sulfur corresponding to the LiCF₃SO₃ from the electrolyte¹⁵ as observed in the case of Figure V – 6b for the commercial separator soaked in the electrolyte. The absence of any detectable polysulfide in the post-cycled separators cycled from electrodes generated with the CFM-1 and CFM-2, especially after 200 cycles (Figure V – 6 (d, e)) indicates complete constriction of the formed polysulfide within the CFM structures possibly due to chemical-binding of S to the CFM architecture as observed in the TEM images (Figure V - 5) and XPS (Figure V - 6). In addition, spatial confinement (Table V – 4) possibly aids in ensuring polysulfide retention at the electrode. Though the porous structures have previously been shown to result in improved cycling behavior, complete masking of polysulfide dissolution using a porous host has seldom or never been reported to the best of our knowledge. The unique cage-like structure of the CFMs along with the chemical binding occurring therein thus results in a very stable cycling performance with a remarkably low fade rate of ~0.0014% cycle⁻¹.

However, both the S-CFM electrodes generated with undergo initial loss in capacity which is typically known to occur and attributed to the polysulfide dissolution. The XPS results discussed above clearly indicate that this loss cannot be related to polysulfide dissolution as evidenced by the lack thereof of any sulfur species detected on the separators [Figure V – 6 (d, e)]. To understand the origin of this initial capacity loss observed, XPS was performed on both the S – CFM coated electrodes before and after 200 cycles. Figure V - 7 represents the C1s spectrum of slurry cast S – CFM electrodes and the same electrodes post cycling. S – CFM-1 (Figure V - 7a) and S-CFM-2 (Figure V - 7c) electrode samples have peaks corresponding to –(CF₂ – CF₂) – bonds from PVdF binder (289.87 eV)²⁰, -C₆H₅S- bond corresponding to ring C – S interactions (285.59 eV)²¹ and –C₆H₄S₂- (284.4 eV)²². The presence of the C-S peaks herein confirms the observations in the S2p spectrum (Error! Reference source not found.) and corroborates the hypothesis that sulfur-carbon bonding aids in ensuring superior polysulfide retention within the CFM structure. The S – CFMs post-200 cycles showed two C1s peaks at 292.41 eV and 289.55 eV in addition to the peaks observed before cycling. The peak at 292.41 eV corresponds to the CF₃SO₃⁻¹⁵ group of the lithium salt LiCF₃SO₃ used with the organic electrolyte. The peak at 289.55 eV corresponds to Li₂CO₃²³ resulting from the irreversible reaction of Li⁺ ions with the –(CO₃)⁻ groups of the CFM.

Figure V – 8 depicts the S2p profiles of the S-CFM electrodes before and after cycling. Both S-CFM-1 and S-CFM-2 electrodes before cycling show S2p peak at 162.45 eV representing the bonding of sulfur to CFMs (as also observed in Error! Reference source not found.). Both S – CFM-1 and S – CFM-2 electrodes post-cycling however, show the presence of a satellite peak at 170.20 eV, corresponding to the occurrence of sulfur-carbon bonding^{21, 24}. This indicates that sulfur is bound to the carbon before cycling as well as through the various stages of cycling preventing the loss of sulfur through polysulfide run-away to bulk electrolyte during cycling resulting in exceptional cycling stability. In addition to the peaks corresponding to

C-S bonding, there are unique peaks observed in the post-cycled electrodes corresponding to the formation of a mixture of sulfate species. The irreversible loss in capacity could thus be attributed to irreversible consumption of sulfur through the formation of lithium, and other sulfates during electrochemical cycling. Thus, deactivation of the active material of sulfur occurs through the formation of sulfate species during the initial cycling resulting in irreversible capacity loss. The results presented herein clearly demonstrate that the embedding of sulfur into the nanoporous CFM frameworks directly in the as-prepared form without any carbonization step ensures minimal polysulfide transport out of the electrode into the separator ensuring minimal capacity loss because: (a) chemical bonding of carbon in the CFM structure with sulfur; and (b) constriction of the lithium polysulfide species within the porous matrix. This is indeed reflected resulting in stable capacity of $\sim 609 \text{ mAh g}^{-1}$ with a fade rate of only $\sim 0.0014\% \text{ cycle}^{-1}$ demonstrating the promise of this novel synthetic strategy. Based on the insight gained from this study sulfur infiltrated framework materials (SFM) with higher ionic conductivities were developed and upon testing showed an initial capacity of 1626 mAh/g with stable performance of 1044 mAh/g for over 100 cycles (Figure V - 9). As an additional subtask of Phase-2, an air – stable inorganic framework material (IFM) was explored to trap polysulfides (Figure V - 10a shows the XRD patterns of S doped IFM). The IFMs exhibit very high (80%) S infiltration and a low irreversible capacity loss of 15%. Further, the IFMs improved the first cycle specific capacity of S to $\sim 1250 \text{ mAh/g}$ stabilizing at $\sim 750 \text{ mAh/g}$ (Figure V - 10b). The improved specific capacity of the sulfur electrode is attributed to the successful polysulfide trapping by IFMs and work is currently on-going to improve the performance further, the results of which will be reported in future reports.

Conclusions:

The aim of *Phase-2* was to establish methods to improve sulfur cycling characteristics by employing interface engineering strategies and use of framework structures. In addition, the work was directed at developing doped LIC materials and doped sulfur nanoparticles. By implementing such approaches various materials have been derived with initial capacities in excess of 1400 mAh/g with retention of $>1000 \text{ mAh/g}$ after 100 cycles. It can also be clearly observed that fade rates have been significantly reduced by using the 4 approaches in *Phase-2* described above. Exceptionally low fade rates of $\sim 0.0014\%$ loss per cycle have been observed and in the case of CFM materials a complete absence of polysulfides at the separator has been shown after 200 cycles. In *Phase-3* of the study, emphasis will be laid on optimization of these systems with the goal of achieving more than 1000 mAh/g for 1000 cycles. Results of these studies will be reported in subsequent reports.

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Figures and Tables Begin on Next Page

Figures and Tables:

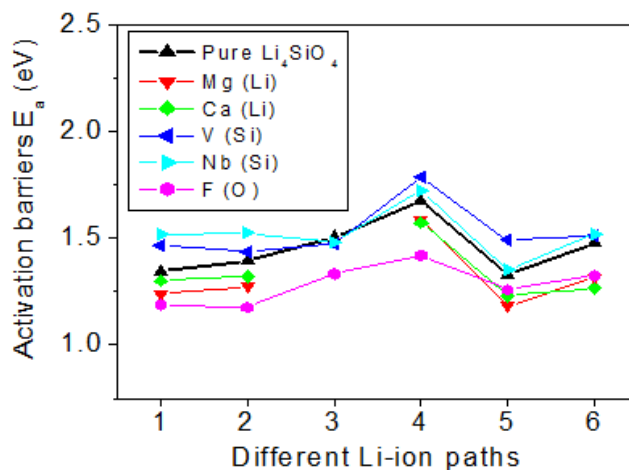


Figure V - 1. Activation barriers E_a (eV) for different migration Paths of Li-ions in pure and doped Li_4SiO_4 .

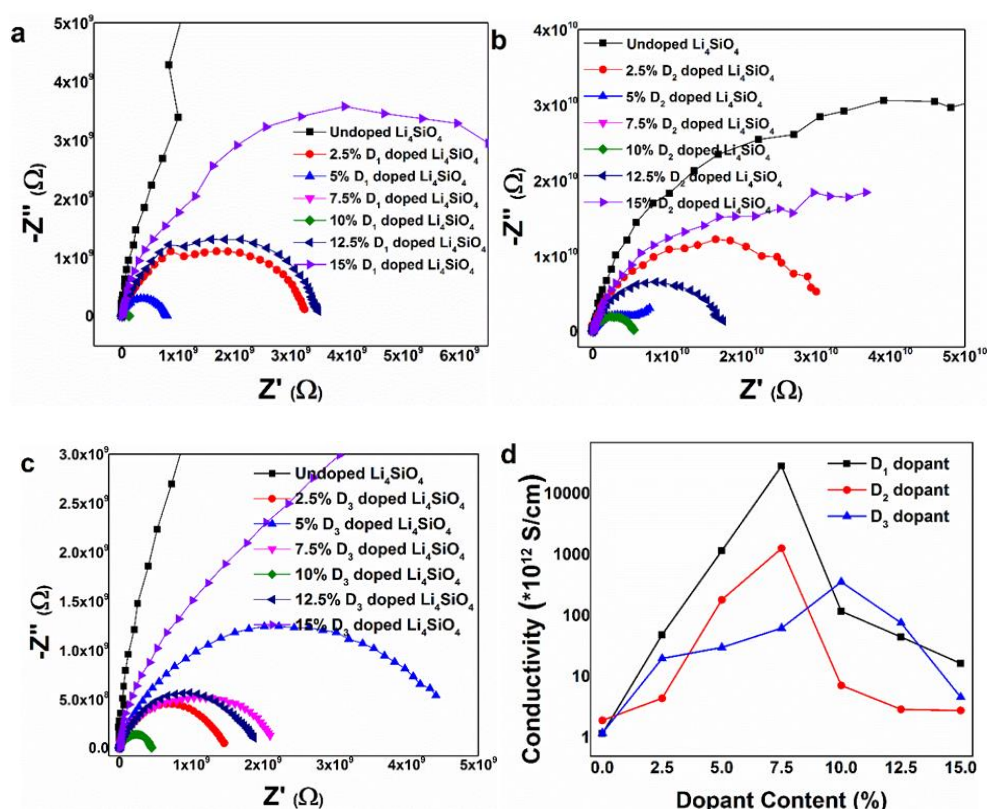


Figure V - 2. a) AC impedance based conductivity analysis of D1 doped Li_4SiO_4 ; b) AC impedance based conductivity analysis of D2 doped Li_4SiO_4 ; c) AC impedance based conductivity analysis of D3 doped Li_4SiO_4 and d) Effect of doping D1, D2 and D3 on the conductivity of Li_4SiO_4 .

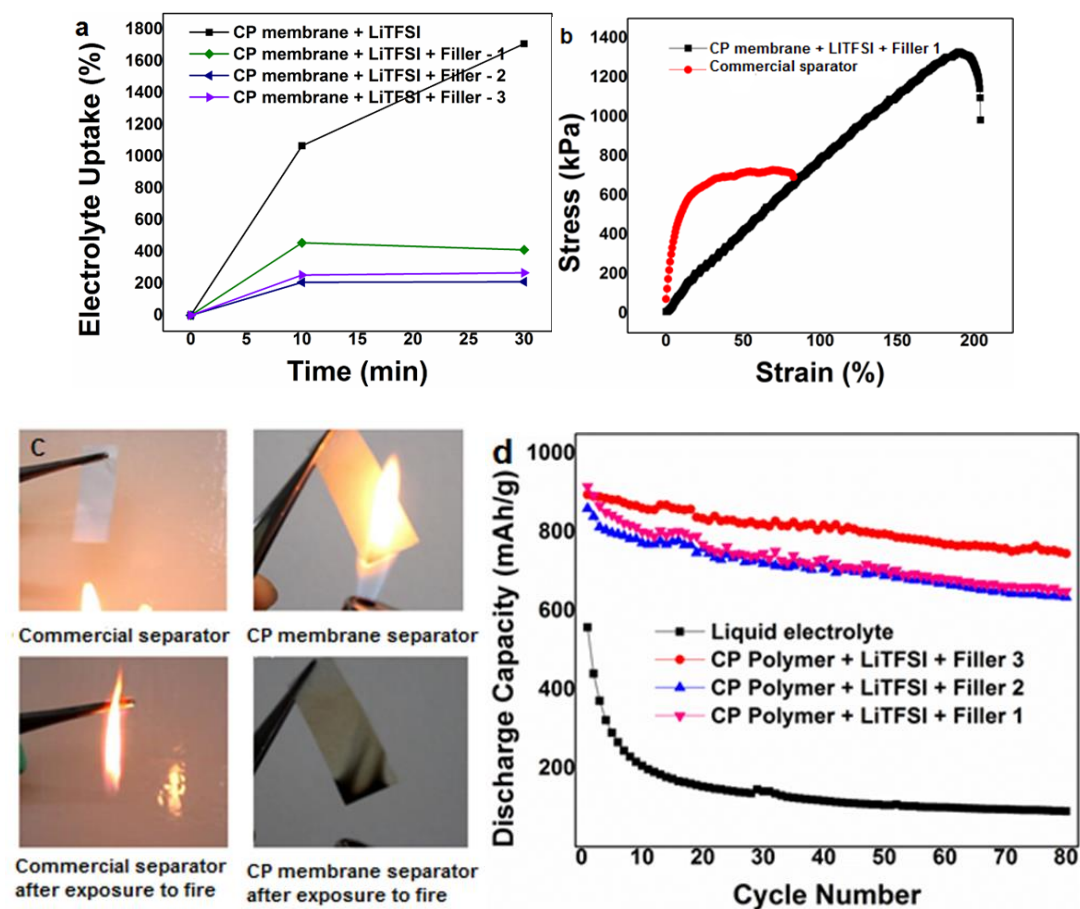


Figure V - 2. (a) Electrolyte uptake of CPE membranes (b) Mechanical properties of the CPE membrane (c) Flame-test depicting the superior safety of the CPE materials (d) Cycling behavior of CPE membranes.

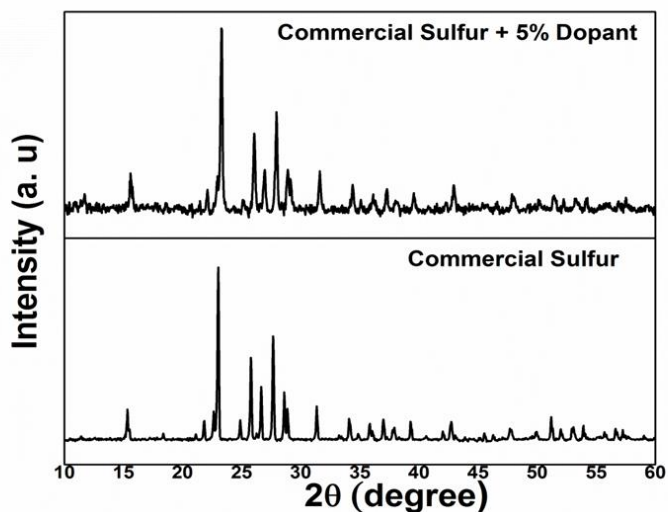


Figure V - 3. XRD pattern of synthesized doped sulfur material showing phase-purity and peak shift.

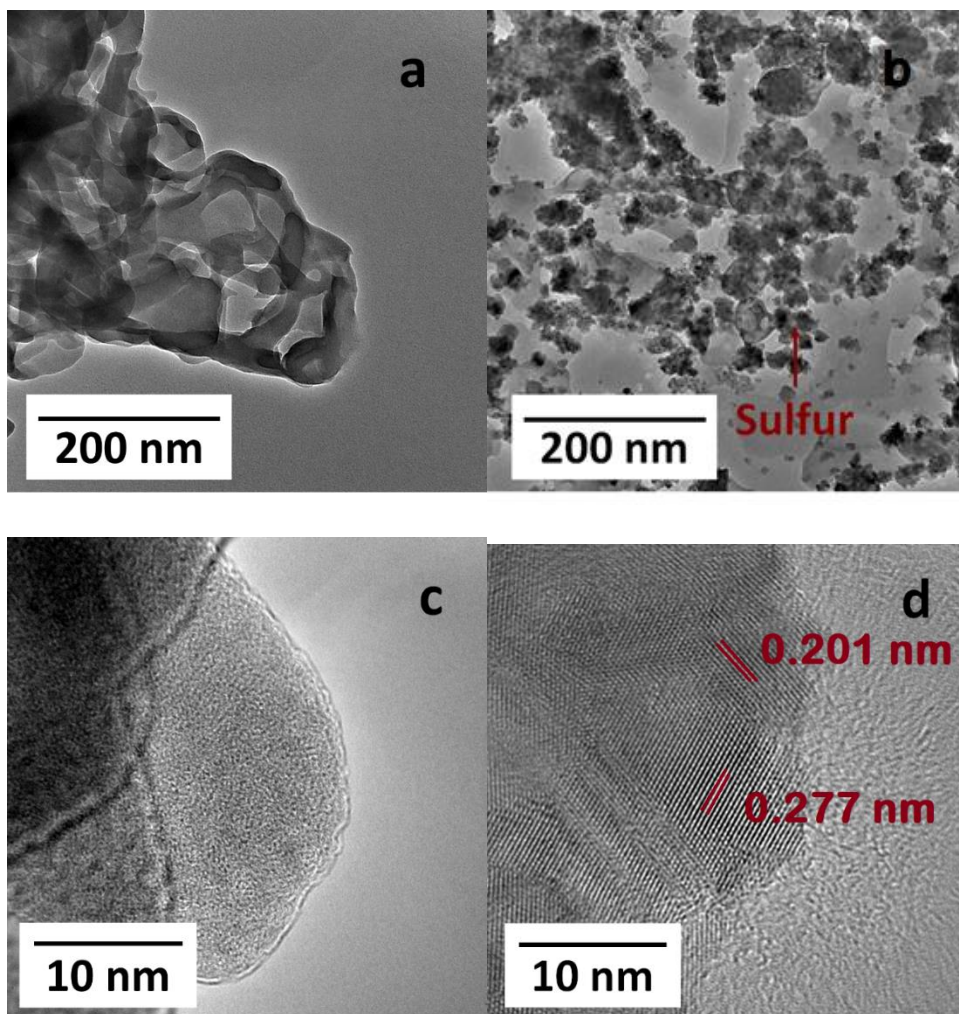


Figure V - 4. TEM images of CFM-1 and S -CFM-1 at different magnifications. (5a, 5c) CFM-1; (5b and 5d) S-CFM-1.

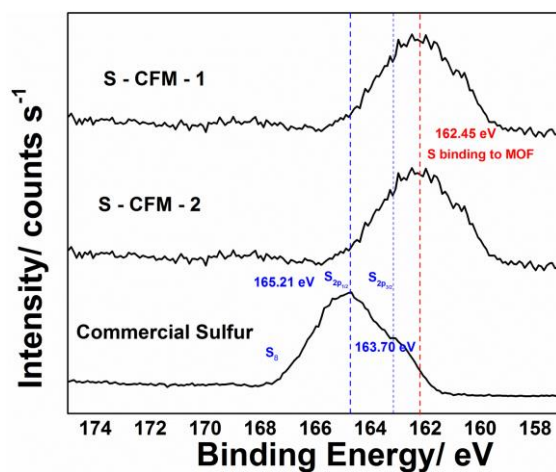


Figure V - 5. XPS S2p Binding Energy profile of Commercial Sulfur, S - CFM-1 and S - CFM-2.

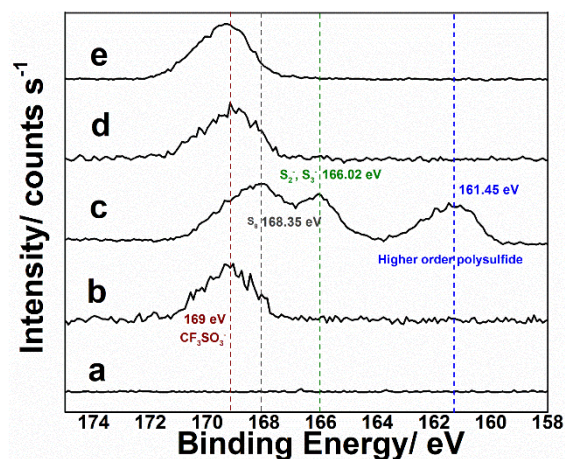


Figure V – 6. XPS S2p binding energy profile of a) commercial separator b) commercial separator soaked in electrolyte; separators of c) commercial sulfur electrode; d) S – CFM-1; e) S – CFM-2 electrodes; (after 200 cycles at 0.2 C rate).

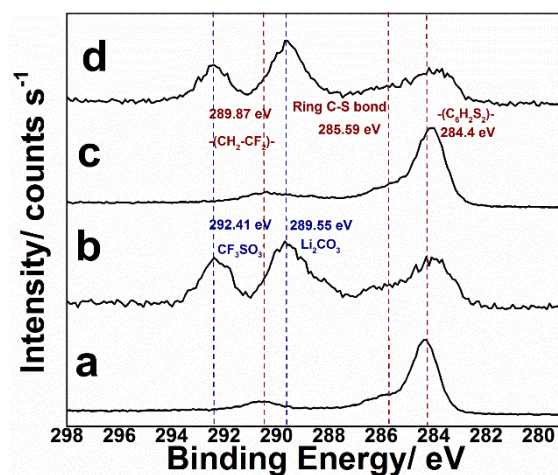


Figure V - 7. XPS C1s Binding Energy profile of slurry coated electrodes of a) S – CFM-1 before cycling, b) S – CFM-1 after 200 cycles, c) S – CFM-2 before cycling, and d) S – CFM-2 after 200 cycles at 0.2 C rate.

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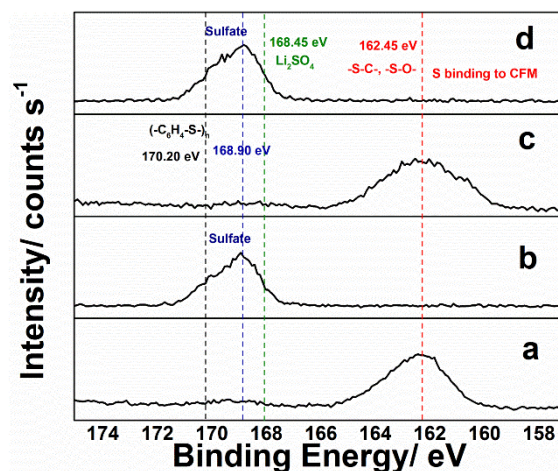


Figure V – 8. XPS S2p Binding Energy profile of slurry coated electrodes of
 a) S – CFM-1-before cycling, b) S – CFM-1 after 200 cycles,
 c) S – CFM-2-before cycling and d) S – CFM-2 after 200 cycles at 0.2 C rate.

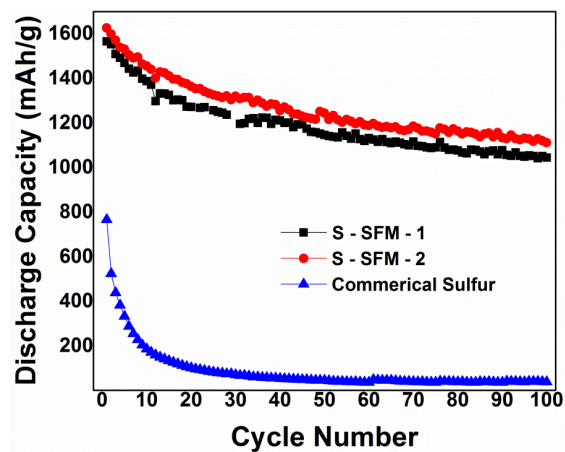


Figure V - 9. Cycling performance of Sulfur-infiltrated Framework Material (SFM).

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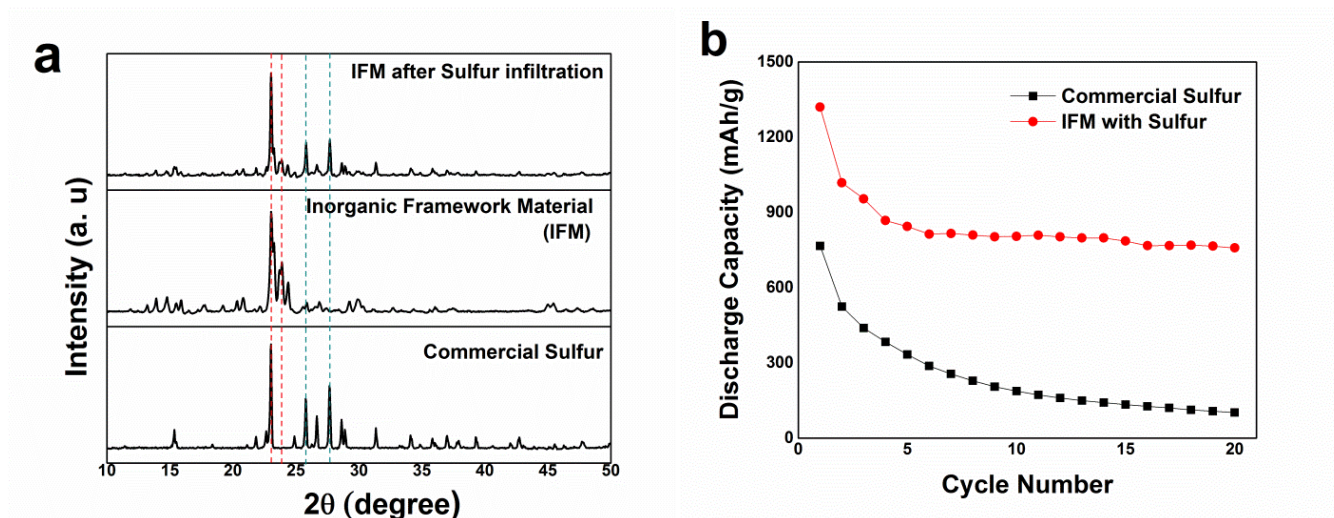


Figure V - 10 (a) XRD patterns showing the infiltration of Sulfur into the Inorganic Framework Material (IFM) showing retention of IFM structure. (b) Cycling behavior of Sulfur infiltrated IFM.

	D ₁ doped ($\times 10^{12}$ S/cm)	D ₂ doped ($\times 10^{12}$ S/cm)	D ₃ doped ($\times 10^{12}$ S/cm)
Li ₄ SiO ₄ – undoped	1.16	1.29	1.19
2.5% doped	49.13	4.44	20.04
5% doped	1169.55	183.51	30.41
7.5% doped	28706.06	1277.59	63.13
10% doped	119.26	7.22	359.62
12.5% doped	45.08	2.93	76.95
15% doped	16.53	2.80	4.66

Table V - 1. Lithium ionic conductivities of Li₄SiO₄ upon doping with three different dopants D₁, D₂ and D₃.

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Sample Composition	Conductivity (S/cm)
Commercial separator with liquid electrolyte	$1.283 \cdot 10^{-3}$
CP membrane + LITFSI + Filler 1	$1.881 \cdot 10^{-3}$
CP membrane + LITFSI + Filler 2	$3.009 \cdot 10^{-3}$
CP membrane + LITFSI + Filler 3	$9.4749 \cdot 10^{-3}$

Table V – 2. Lithium ion conductivities of commercial separator compared with composite polymer membranes with three different fillers.

Mechanical properties	CP membrane separator	Commercial separator
Tensile strength (kPa)	1114.8	636.1
Elongation break (%)	107.9	95.2
Young's modulus (GPa)	11.8	10.6

Table V - 3. Comparison of the mechanical properties of CP membrane and commercial separator.

	BET Surface Area/ $\text{m}^2 \text{g}^{-1}$	Langmuir Surface Area/ $\text{m}^2 \text{g}^{-1}$	Total Pore Volume/ $\text{cm}^3 \text{g}^{-1}$	Adsorption average pore width/ nm
CFM-1	525.98	829.18	0.324	2.46
CFM-2	684.25	1083.07	0.422	2.47

Table V – 4. BET surface area analysis of two different types of CFMs.

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AVPTA Technology Focus Area 6: Energy Storage and Batteries

High Fidelity Fast Running Multiscale Multiphysics Battery Pack Software

DOE-VTO TFA Lead: David Howell
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Project Start: Q2FY16
Estimated Completion: Q3FY2019

Objective(s):

GH-MSMD Extension and Implementation:

- To enhance and extend the computationally efficient modular multi-scale multi-domain (MSMD) battery model framework that integrates physicochemical processes occurring in wide-range time and length scales spanning from particles to battery packs and resolves the nonlinearity of physics models with proper spatial resolution.
- To implement it in the commercially available software, FLUENT, both at the cell-level and pack-level, using a new partially linearized quasi-explicit “GH” model technique.

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Linear ROM Development:

- The objective of this task is to enhance and extend the linearized reduced-order model concepts to improve their flexibility to handle variations. This task is composed of two parallel subtasks as follows:
 - Parametric macro-modeling
 - ANSYS will research and develop new approaches based on FLUENT results that avoid the need to rebuild the ROM due to:
 - (a) Time-varying battery coolant flow rate
 - (b) Time- and space-varying electrochemical heat sources
 - Response-surface ROM
 - ANSYS will extend the response-surface concept in DesignXplorer to generate a battery ROM that includes geometric parameter variations and can:
 - Generate fast stand-alone results to support preliminary design optimization
 - Be embedded as a component model into transient system simulations

Nonlinear ROM Development:

- The objective of this task is to continue the research on the discrete empirical interpolation method to create nonlinear ROMs for both the cell and electrode domains. This task is composed of two subtasks that are reasonably independent but are planned sequentially due to resource limitations.
 - DEIM for CDM
 - ANSYS and ESim will build on the results of CAEBAT I to develop DEIM for the cell domain model (CDM).
 - DEIM for EDM
 - ANSYS and ESim will research DEIM as an option for the electrode domain model (EDM).

Interactive System Interface Development and Evaluation:

- The objectives of this task are to build a capability to run a 3D battery pack simulation interactively with inputs from other components in the system without sacrificing computational speed.

Development of Evolving Performance Model Against Usage and Stress Factors:

- The objective of this task is to enhance and extend the equivalent circuit life model developed in CAEBAT I, and to develop a P2D life model. This task consists of two subtasks.
 - ECM Life Model
 - ESim will work with ANSYS and GM to incorporate the ECM life model developed in CAEBAT I into ANSYS software. This model will also be extended to include capacity fade due to loss of active material from the anode and the

cathode by using a natural decay equation as presented by Rahimian et al.[JES, 159, A860]

– P2D Life Model

- ESim will work with ANSYS and GM to develop a P2D life model for use in ANSYS. This model will be used to develop synthetic data for arbitrary vehicle drive and storage cycles. This synthetic data will then be used for example as the data for fitting the ECM life model developed in Subtask 5.1. This model will include capacity fade due to formation of the SEI layer on the anode particles, loss of active material from the anode and the cathode and other mechanisms as needed to simulate the materials of a particular lithium ion cell. The reduced order model presented by Guo and White [9] will be considered for use in this model. Also the reduced order models produced in other tasks in this project will be incorporated into this P2D life model.

Strategic Context:

Energy storage system based on lithium-ion batteries is promising to improve the energy efficiency and functionality of military vehicles through electrification. TARDEC is interested in enhancing and utilizing computer tools to accelerate development and fielding safe, high-performance, and long-lasting lithium ion battery module for military vehicle applications. The tool should be capable of accurately predicting cell and module multiphysics behaviors occurring across a wide range of scale to help the design and evaluation of the batteries in military vehicle environment.

Accomplishments:

Due to an inordinate delay of almost a year in the sub-recipient contract signing between GM and ANSYS, only a fraction of the *Tasks 1, 2, 3 and 4* mentioned above in the objectives section were accomplished during 2016. Despite this delay, following are the key accomplishments for this year:

- NREL ran benchmark comparison cases between GH-MSMD and full-MSMD with excellent agreement between the two results, and has submitted the GH-MSMD paper on Sept-30, 2016 to the Journal of Electrochemical Society.
- NREL developed and demonstrated a TUI (Text-User-Interface) to drive the MSMD and GH-MSMD simulations interactively from the command line in FLUENT. This was accomplished through a collection of multiple text commands available in FLUENT 16.0 in a journal file. This satisfied one of the goals in *Task 4* “Identify TUI procedure for running MSMD simulation in FLUENT”.
- During the 1st quarter of 2016, ESim LLC put together some fundamental research work which can be used as the basis for the development of a physics-based life model for Li-ion cells. This baseline work includes:
 - An updated Pseudo-2D model for a Li-ion cell in which the capacity fade mechanism due to SEI side reaction at the anode was added.
 - The accuracy of the Pseudo-2D life model was validated by comparison to the cycling data with several different protocols

- During the 2nd quarter of 2016, ESim LLC reformulated the pseudo-2D model of Li-ion battery into a space-space model and derived a solution algorithm based matrix-exponential method. Compared with the physics-based PDE formats, this reformulated pseudo-2D model is more suitable to be used for online parameter estimation with high-frequency data sampling.

Introduction:

To accelerate the production of safe, reliable, high-performance, and long-lasting lithium-ion battery packs, the automotive industry requires computer-aided engineering (CAE) design tools that accurately represent cell and pack multi-physics phenomena occurring across a wide range of scales. However, due to the lack of battery pack engineering software providing the desired computational speed, flexibility, and solution accuracy, current design and development of automotive battery pack systems heavily rely on costly and time consuming experimental tests. For example in battery life estimation, GM has instituted multi-parameter Design of Experiments generating test data at cell level and pack level on a reduced basis for each hybrid vehicle program. Generating test data on a pack level has been found to be very expensive, resource intensive, and sometimes unreliable. If a high fidelity fast running multi-physics battery pack model is available, we expect that a model-based approach will replace a significant portion of pack-level aging experiments and reduce 300 pack test-weeks per program.

Physicochemical processes in lithium ion batteries occur in intricate geometries over a wide range of time and length scales. As the size of the battery increases, macroscopic design factors in combination with highly dynamic environmental conditions significantly influence the electrical, thermal, electrochemical, and mechanical responses of a battery system. NREL pioneered the MSMD model, overcoming challenges in modeling the highly nonlinear multi-scale response of battery systems. The MSMD model provides flexibility and multi-physics expandability through its modularized architecture. The project team previously collaborated on combining new and existing battery models into engineering simulation software that provides 3-D battery pack simulation modeling capability. Because of increasing complexities when configuring additional electrical and thermal connections between the cells, the computational cost of simulating a battery pack response is still high: results take weeks, unless low-fidelity sub-models are used to represent the battery's current/voltage response. Therefore, substantial improvement of computational efficiency is needed. Software tools also need improved usability and flexibility to reduce both the computational time and the engineering labor required to keep pace with battery design changes, including geometry and configuration. These improvements would enable the use of models in design and management tradeoff studies of performance/life in large vehicle battery pack systems, which are typically composed of several hundred large-format individual cells.

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Approach:

The project is designed to achieve the suggested project objectives through two parallel phases with six tasks:

Phase-1 - Enhance Computation Speed and Stability of Pack-Level Multi-Scale Model:

- *Task 1.* GH-MSMD extension and implementation
 - Subtask 1.1: Cell-level implementation
 - Subtask 1.2: Pack-level extension and implementation
 - Subtask 1.3: Implementation verification
- *Task 2.* Linear ROM development
 - Subtask 2.1: Parametric macro-modeling
 - Subtask 2.2: Response-surface ROM
- *Task 3.* Nonlinear ROM development
 - Subtask 3.1: DEIM for CDM
 - Subtask 3.2: DEIM for EDM

Phase-2 - Enhance Multi-Physics Integrity at Pack-Level to Enable Model-Based Diagnostics and Prognostics:

- *Task 4.* Interactive system interface development and evaluation
 - Subtask 4.1: TUI-driven interactive MSMD simulation
 - Subtask 4.2: TUI-driven interactive GH-MSMD simulation
- *Task 5.* Development of evolving performance model against usage and stress factors
 - Subtask 5.1: ECM-based life model enhancement and implementation
 - Subtask 5.2: P2D-based life model enhancement and implementation

Results and Discussion:

During BP1 (Budget Period 1) for *Task-1*, NREL ran benchmark comparison cases between GH-MSMD and full-MSMD, shown in Figures 1-3.

As can be seen from these Figures (1-3) there is an excellent agreement between full-MSMD and GH-MSMD.

For *Task-4* NREL identified TUI procedure for running MSMD simulations using text-driven functions arranged in a FLUENT's 'journal' file as shown below in Figure 4. Figures 5-6 show temperature and potential distribution after 180 seconds of discharge using TUI simulations.

The following sections pertain to the results obtained in *Task-5* "Development of evolving performance model against usage and stress factors for physics-based life model" carried out by ESim LLC.

During the 1st quarter of 2016, ESim LLC put together some fundamental research work which can be used as the basis for the development of a physics-based life model for Li-ion cells. This baseline work includes:

- An updated Pseudo-2D model for a Li-ion cell in which the capacity fade mechanism due to SEI side reaction at the anode was added.
- The accuracy of the Pseudo-2D life model was validated by comparison to the cycling data with several different protocols

To develop the Pseudo-2D life model, the mechanism for the anode SEI reaction was coupled with the physics-based model equations. The current density for the SEI formation at the surface of anode, j_s , is expressed as follows:

$$j_s = i_{0,s} \exp \left[-\frac{\alpha_s n_s F}{RT} (\phi_1 - \phi_2 - U_s + j_a R_{\text{film}}) \right] \quad (1)$$

where $i_{0,s}$ is the pre-exponential exchange current density for SEI side reaction, α_s is the symmetry coefficient, n_s is the number of electrons transferred in the reaction, F is the Faraday constant, R is universal gas constant, T is temperature, ϕ_1 is the electrical potential of solid-phase, ϕ_2 is the electrical potential of solution-phase, U_s is the equilibrium potential of the SEI side reaction, j_a is the current density for the intercalation of Li-ions at the surface of anode, and R_{film} is the resistance of SEI film. The SEI film grows with the side reaction:

$$\frac{d\delta_{\text{film}}}{dt} = \frac{j_s M_{w,\text{film}}}{n_s F \rho_{\text{film}}} \quad (2)$$

where δ_{film} is the thickness of SEI film, $M_{w,\text{film}}$ is molecular weight of SEI film, and ρ_{film} is the density of SEI film. The SEI film resistance is expressed as follows:

$$R_{\text{film}} = \frac{\delta_{\text{film}}}{\kappa_{\text{film}}} \quad (3)$$

where κ_{film} is the conductivity of the SEI film.

The test data for model validation were collected from Li-ion cells (labeled as LIB4 LIB6, and LIB7) cycled with three different protocols. The key parameter values for the Pseudo-2D model (i.e., solid phase diffusivities and reaction rate constants) were estimated by fitting the model with the voltage and current data at the beginning of life. The profiles for data vs model comparisons are presented in Figure-7.

The key parameters for these cells were estimated by fitting the model to data and are the values listed in Table 1, these values are held constant for all the three cells through all of the cycles.

After initial validation, the Pseudo-2D model was run for cycling simulation, the predicted capacity vs cycle profiles were compared with cycling data, and the results are shown in Figure-8.

To fit the capacity fade model to life profiles, two groups of parameters were used. The first group (see Table 2) includes parameters for the SEI reaction, and these physics-related parameters are the same for all cells.

Another group (see Table 3) includes parameters related to the cell design, and cell-to-cell variations are included.

During the 2nd quarter of 2016, ESim LLC reformulated the pseudo-2D model of Li-ion battery into a space-space model and derived a solution algorithm based matrix-exponential method. Compared with the physics-based PDE formats, this reformulated pseudo-2D model is more suitable to be used for online parameter estimation with high-frequency data sampling.

The Reformulation of Pseudo-2D Model:

A summary of the governing equations for the pseudo-2D model is shown in the following Table 4.

Normally, the equations listed in Table 4 are solved by software tools with a nonlinear DEA solver, and the input variable should be pre-defined with smooth profiles (i.e. constant current/power). In the online control mode, however, the input signals to a battery usually vary rapidly with time in a non-smooth pattern. Figure 9 shows the profile for the input current signal to battery during a typical drive cycle.

To implement the pseudo-2D model into the high-frequency operation mode, the governing equations should be translated into a state-space model. After geometry meshing, the mass transfer equations (both solid and electrolyte phases) can be written as follows:

$$\dot{\underline{\mathbf{c}}} = - \underline{\underline{\mathbf{K}}} \underline{\mathbf{c}} + \underline{\mathbf{f}} \quad (4)$$

where $\underline{\mathbf{c}}$ is the discretized concentration vector, $\underline{\underline{\mathbf{K}}}$ is the stiffness matrix, and $\underline{\mathbf{f}}$ is the loading vector. From time t_{k-1} to t_k , the concentration values are updated by the following equation:

$$\underline{\mathbf{c}}_k = \exp\left[-\underline{\underline{\mathbf{K}}}_{k-1} (t_k - t_{k-1})\right] \underline{\mathbf{c}}_{k-1} + \underline{\underline{\mathbf{K}}}_{k-1}^{-1} \left\{ \underline{\mathbf{I}} - \exp\left[-\underline{\underline{\mathbf{K}}}_{k-1} (t_k - t_{k-1})\right] \right\} \underline{\mathbf{f}}_{k-1} \quad (5)$$

where the subscript k denotes the index of the time step. The charge conservation equations can be described by algebraic constraints shown as follows:

$$F(\underline{\mathbf{c}}_k, \underline{\mathbf{f}}_k, I_k, V_k) = 0 \quad (6)$$

where I_k is the current input and V_k is the voltage response of battery. Due to the nonlinearity of the Butler-Volmer equation, the algebraic constraints (3) must be solved iteratively and thus slow down the computation procedure. However, by taking proper simplification of equation (6), the voltage response V_k can be obtained as an explicit function of $\underline{c}_k$ and I_k :

$$V_k = h(\underline{c}_k, I_k) \quad (7)$$

Half-Cell Model:

To avoid complexity, the reformulated pseudo-2D model described by equations (4) through (7) was first implemented for a half cell, where a cathode is set as the working electrode and lithium metal as the counter electrode. As this model is expected to be applied for online parameter estimation, its performance is checked by fitting to the synthetic HPPC data generated by a full-order COMSOL model. Random noise of $\pm 20\text{mV}$ was added to the synthetic voltage data (Figure-10).

A flowchart for parameter estimation is shown in Figure 11, the diffusivities of solid and electrolyte phases (D_s and D_l) and the reference-state exchange current density ($i_{a,\text{ref}}$) were optimized in order to fit the model to the data. The initial guesses were set to deviate from true values by 1~2 orders of magnitude.

Comparisons between the model predictions and the data are shown in Figure 12, the optimized model shows good agreement with the synthetic data.

The convergence plots for parameters in each case are shown in Figure 13. The parameter values converge within 10 iterations. The optimized parameter values may differ from the true values by up to 20%. The reason for this deviation can be due to:

- Random noise added to the error in synthetic data;
- Model simplification causes slight loss of accuracy
- Inaccuracy in computing the numerical Jacobin matrix

During the 3rd quarter of 2016, the pseudo-2D model of Li-ion battery was formulated into a nonlinear state variable model (NSVM) with multiple inputs (current and temperature). The solution algorithm for NSVM was optimized so that the simulation speed was increased by 60 times as compared with the full-order COMSOL model.

The Reformulation of Pseudo-2D Model:

The Li-ion cell sandwich (Figure 14) contains dual insertion porous electrodes separated by an ionically conducting separator, and the porous electrodes are formed by spherical insertion particles

In the NSVM, the transport phenomena in the solid and electrolyte phases can be expressed by the following state equation:

$$\dot{\underline{x}} = \underline{Ax} + \underline{Bd} \quad (8)$$

where $\underline{x}$ is the state variable vector, $\underline{A}$ and $\underline{B}$ are coefficient matrices, and $\underline{d}$ is the source vector. The charge conservation and electrochemical kinetic equations can be written into the following non-linear algebraic constraint:

$$\begin{bmatrix} \underline{d} \\ y \end{bmatrix} = F(\underline{x}, \underline{u}) \quad (9)$$

where $\underline{u}$ is the input signal including current and temperature ($\underline{u} = [i_{app}, T]$) and y is the output signal defined as the terminal voltage ($y = V_{ex}$). The flowchart for the solution procedure of NSVM presented in 15 can be described as following steps:

- 1) At the initial time point ($k = 0$), the state vector $\underline{x}_k$ equals to the preset initial values;
- 2) Evaluate the coefficients and operators in the model with $\underline{x}_k$ and $\underline{u}_k$;
- 3) Solve equation (1) to obtain $\underline{d}_k$ and y_k
- 4) Update the index $k = k + 1$;
- 5) Calculate $\underline{x}_k$ from equation (1) using $\underline{d}_{k-1}$ and $\underline{x}_{k-1}$;
- 6) Repeat steps 2) through 5).

The algebraic constraint can be solved by either implicit or explicit approaches; for implicit approach, the Butler-Volmer equations are solved iteratively by Newton's method; for explicit approach, an approximated hyperbolic equation was used to obtain the potential values.

Simulation Results:

The synthesized input signals are presented in Figure 16, the maximum discharge current rate is 2.5C and cell temperature rises from 25°C to 45°C.

A full-order COMSOL model was developed as baseline, and the simulation results of NSVM are validated by the baseline model. The profiles for simulated terminal voltage are plotted in Figure 17.

The implicit NSVM requires 8.95 sec to simulate this drive cycle (2.0msec per solution) and the explicit NSVM requires 8.50 sec (1.9msec per solution). There is very little difference between the two NSVM versions in terms of simulation speed, so the iterative loop for the implicit model does not necessarily add to the computational load. However, the COMSOL model requires 555 sec (124msec per sample) to process this simulation on the same PC, so the NSVM achieves a 60:1 speedup. The absolute error plotted in Figure 18 show that the NSVM has three-digit agreement with the rigorous model.

The cell distributed properties (electrolyte concentration, electrolyte potential, and surface reaction current density) simulated by the NSVM are presented in Figure 19.

The full cell NSVM model can also be used to estimate cell parameter values. In this work, the solid phase diffusivities and reaction rate constants at reference temperature are chosen as adjustable parameters. The initial guesses for these parameters are set 10 times greater than

the true values (ref 1), the NSVM is called by MATLAB for nonlinear regression to fit the baseline model results. The curve fitting results are shown in Figure 20.

The estimated parameter values are listed in Table 5, as shown in these results, the optimized values have slight deviation from the true values. This issue is caused by the over-optimization: due to model-to-model difference, the NSVM deviates from the baseline model even using the same true parameter sets, the nonlinear fitting algorithm will further adjust parameter values to reach the minimum error.

Future Work:

The NSVM approach can be used to solve pseudo-2D model of Li-ion cell with high accuracy and high simulation speed. This approach also applies for nonlinear estimation of cell parameter where slight error is caused by over optimization. In the future, cell capacity fading during cycles will be modeled, and the NSVM approach will be used for life studies.

Conclusions:

Despite a delay of almost a year in the signing of the sub-recipient agreement between GM and ANSYS, and latter's strict stance on not participating in the project work until the agreement is signed, a significant portion of the objectives was accomplished. GM has applied for a 'no-cost' extension of nine months to the DOE. This will help ANSYS in achieving the project targets and objectives for which they are responsible.

Reference:

1. G.-H. Kim, K. Smith, J. Lawrence-Simon, C. Yang, "Efficient and Extensible Quasi-Explicit Modular Nonlinear Multiscale Battery Model: GH-MSMD," *Submitted to J. Electrochemical Society*.

Figures and Tables:

Figures and Tables Begin on Next Page

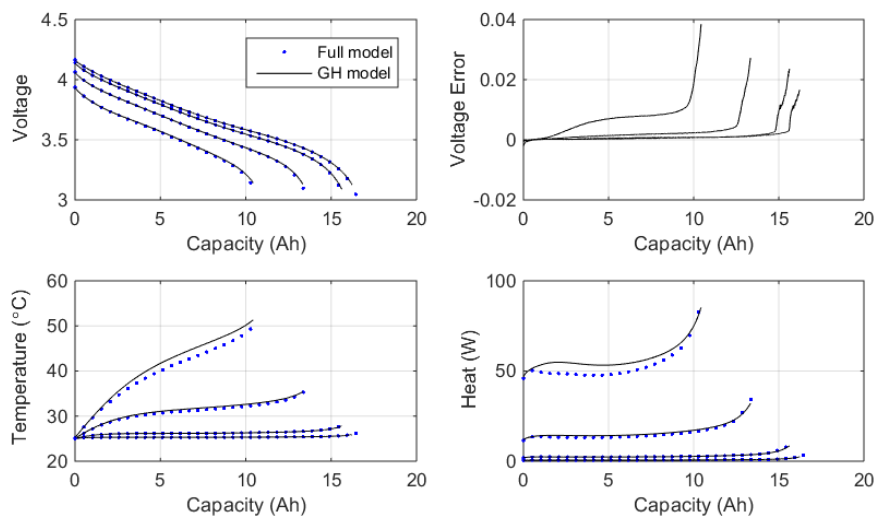


Figure 1. Constant current discharge at 25oC and 1C,2C,5C,10C rates.

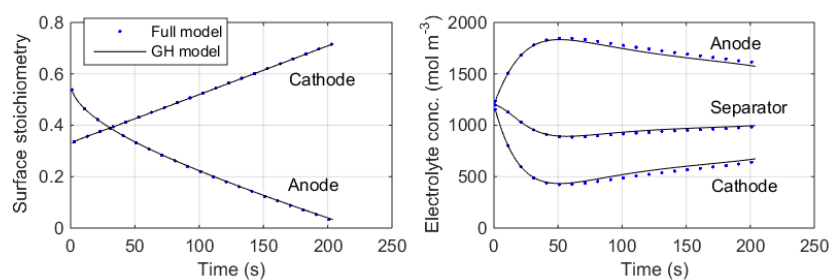


Figure 2. Constant current discharge at 25oC and 10C rate.

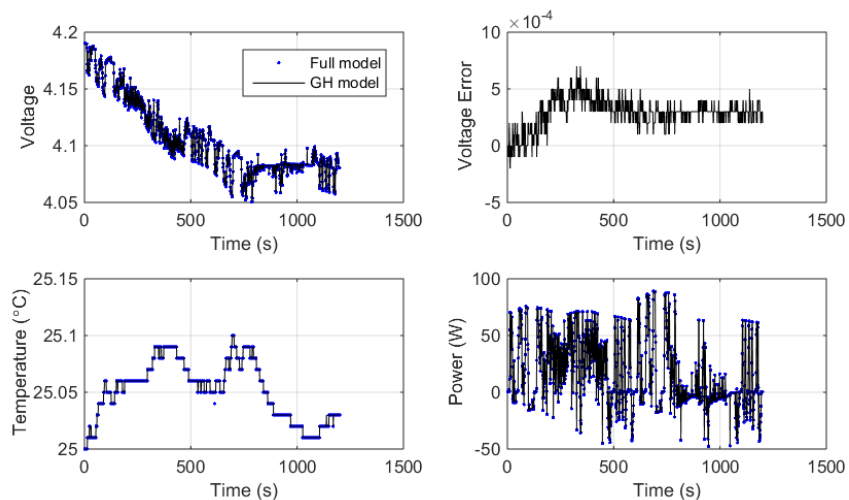


Figure 3. Electric vehicle drive cycle at 25oC.

```

TUI Setup_FV16_1.jou - Notepad
File Edit Format View Help

:Journal file created by cyang!

-----
:--read mesh files--
-----

File>read-case C:\Users\cyang\Desktop\Project2015\MSMD_FOA_AOP_16\TUI_Interface\singlecell\p31ah.msh

-----
:--Case Model Setup: Energy model and Battery Model, without Flow Model--
-----

define/models/unsteady-2nd-order y
define/models/energy y y y
define/models/addon-module 8
define/models/battery-model/enable-battery-model y

-----
:--Setup MSMD Battery Model (NTGK Example)--
-----

MSMD -NTGK Model First Tab
define/models/battery-model/model-parameter y y 31.0 0 0 3000.0 0 3.0 2.4 4.5
: MSMD -NTGK model Second tab
define/models/battery-model/ntgk-parameter/ef-capacity 14.6
define/models/battery-model/ntgk-parameter/u-coefficients 4.12 -0.804 1.075 -1.177 0 0
define/models/battery-model/ntgk-parameter/t-coefficients 1800 -0.00095
define/models/battery-model/ntgk-parameter/y-coefficients 1168.59 -8928 52504.6 -136231 158531.7 -67578.5
: MSMD -NTGK model Third and Fourth Tab
: use " " in tui represents "Enter" key
define/models/battery-model/electric-field-model/current-tab 15 ,
define/models/battery-model/electric-field-model/voltage-tab 14
define/models/battery-model/electric-field-model/conductive-regions 10 , , 8 9 , no

-----
:--Load Material database and Assign cell Zone Materials--
-----

define/materials/data-base/database-type user-defined "C:\Users\cyang\Desktop\Project2015\MSMD_FOA_AOP_16\TUI_Interface
define material copy solid neg_tab
define material copy solid pos_tab
define boundary-condition solid cl_neg_tab yes neg_tab
define boundary-condition solid cl_pos_tab yes pos_tab
define boundary-condition solid cell1 yes cell1

mesh/modify-zones/slit-interior-between-diff-solids

-----
:--battery model update--
-----

(clear-battery-model)
(setup-battery-model)
(set-battery-sources)
(change-to-addon-diffusivity)
(models-changed)

```

Figure 4. Example TUI file for running MSMD simulations in Fluent.

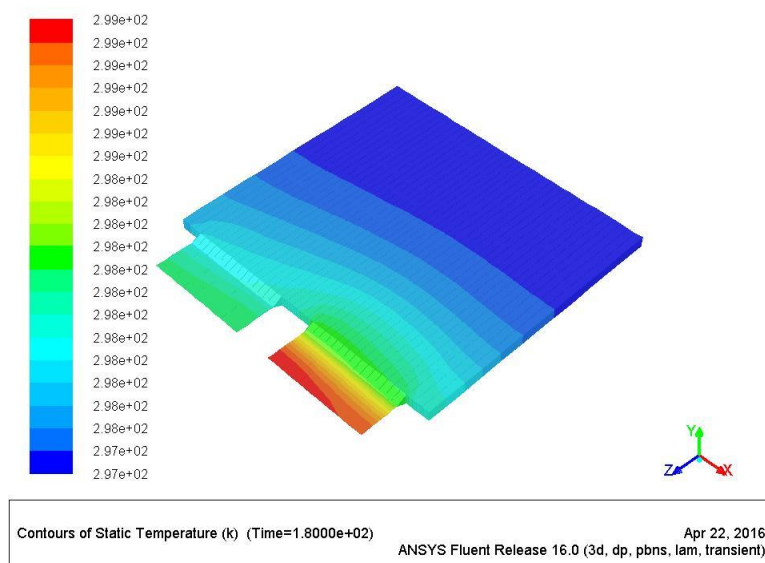


Figure 5. TUI simulation temperature distribution after 180 sec of discharge.

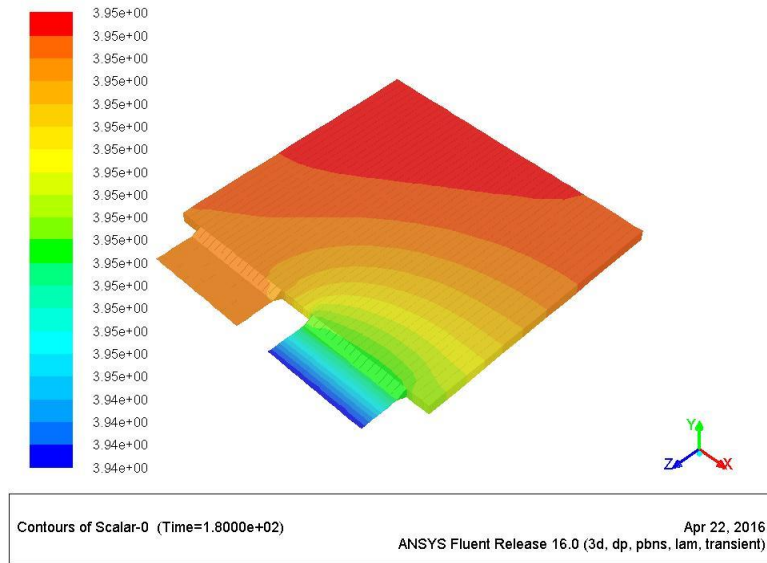


Figure 6. TUI simulation potential distribution after 180 sec of discharge.

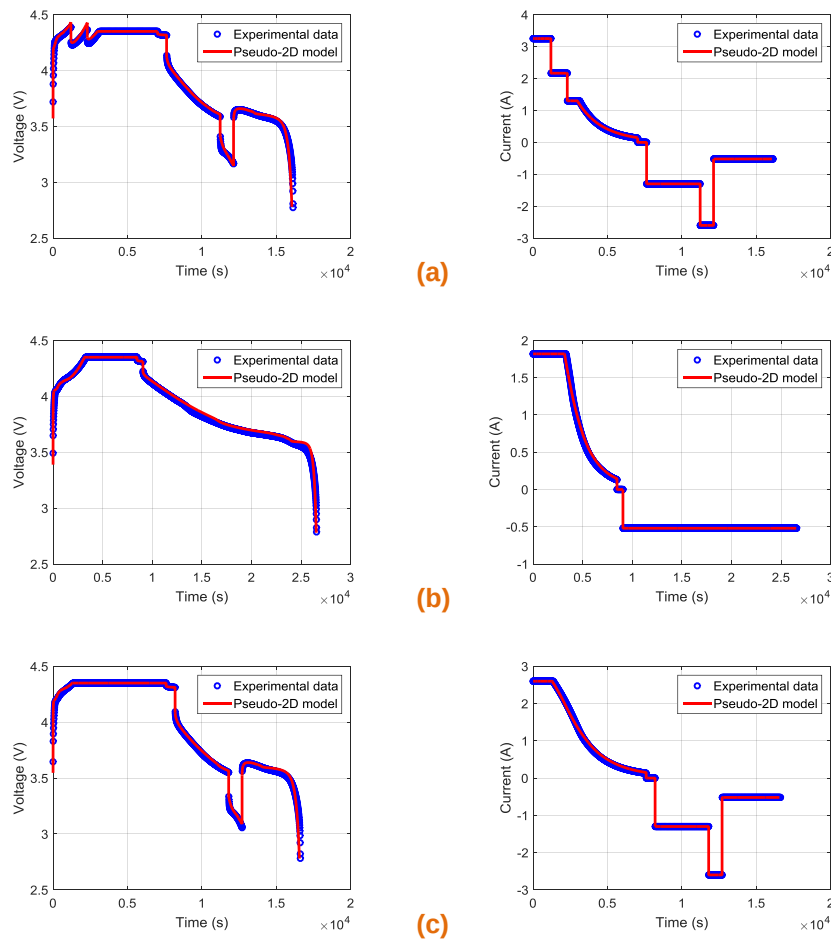


Figure 7. Voltage and current profiles for cells at the initial cycle: (a) LIB4, (b) LIB6, (c) LIB7

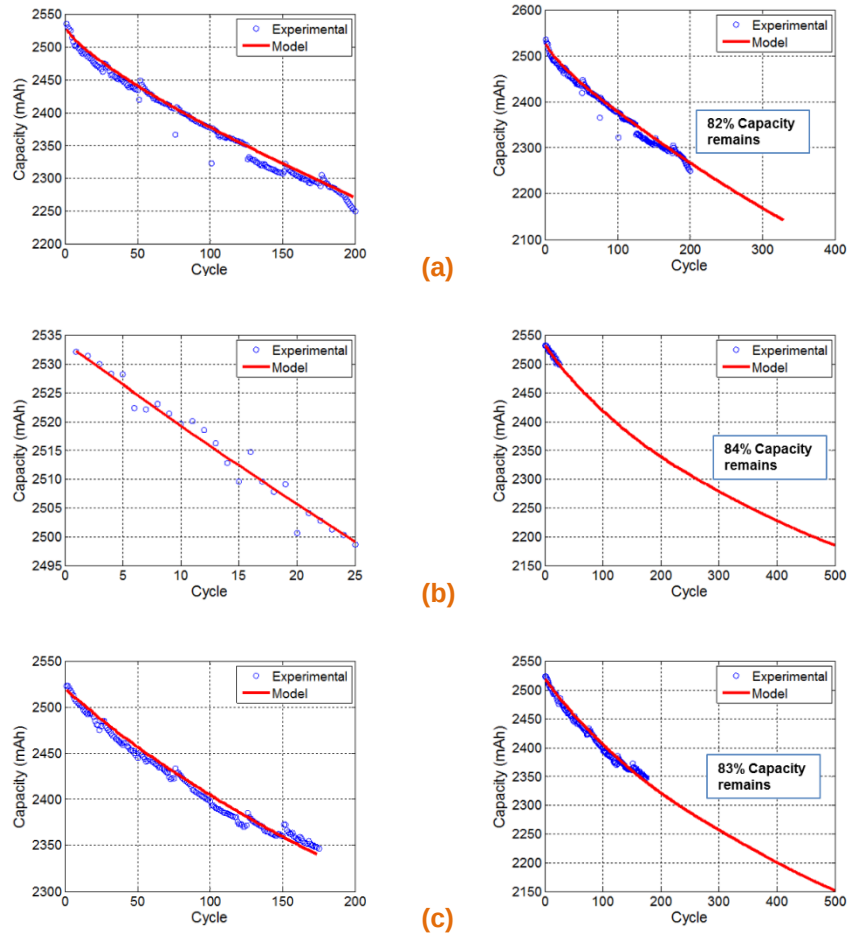


Figure 8. Predicted vs experimental cycling profiles with remaining life prediction for three cells:

- (a) Cycling profile fitting (left) and remaining life prediction (right) for LIB4,**
- (b) Cycling profile fitting (left) and remaining life prediction (right) for LIB6, and**
- (c) Cycling profile fitting (left) and remaining life prediction (right) for LIB7**

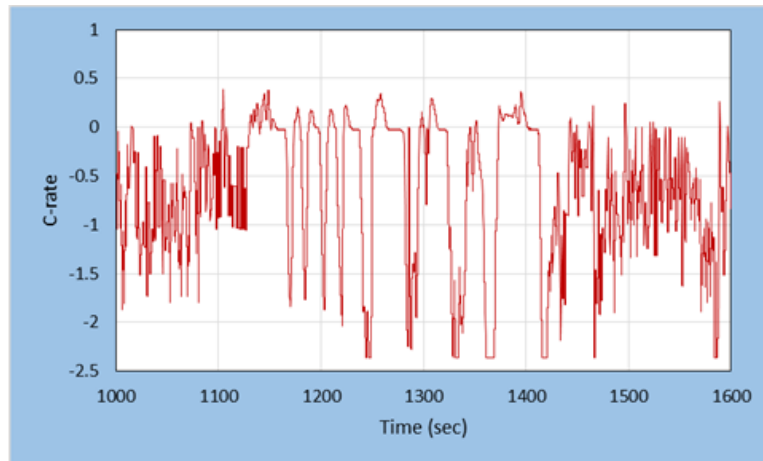


Figure 9. Current profile during a practical drive cycle

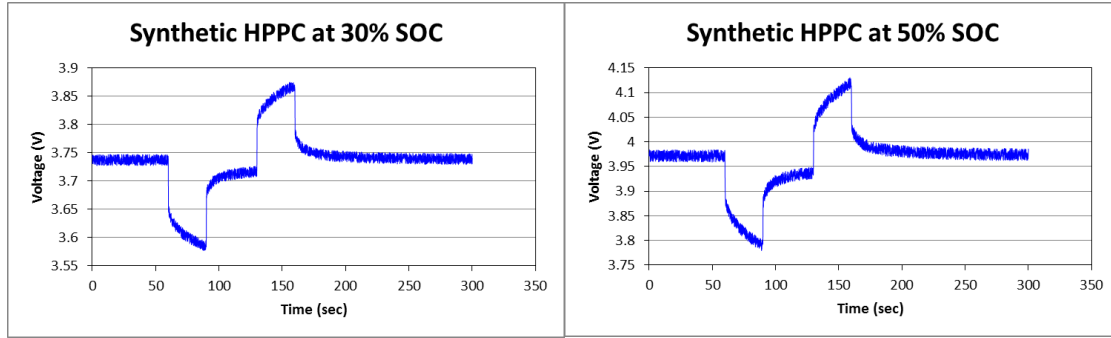


Figure 10. Synthetic HPPC data at 30% & 50% State of Charge (SOC)

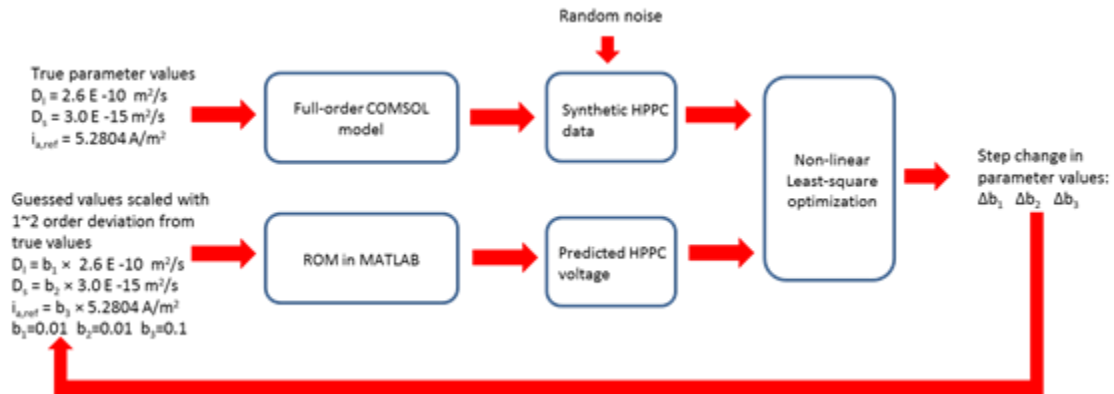
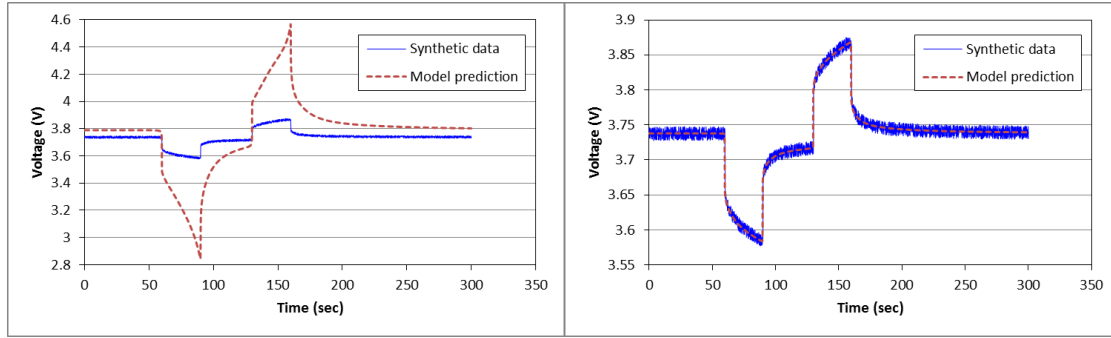
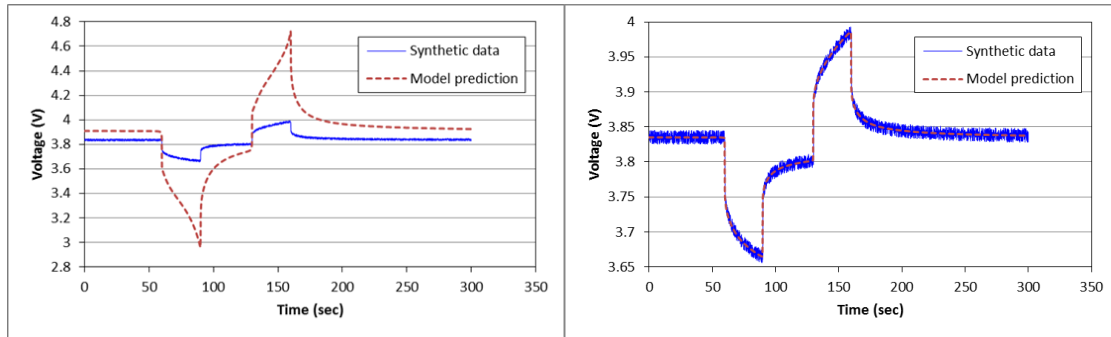


Figure 11. Parameter estimation for half-cell model

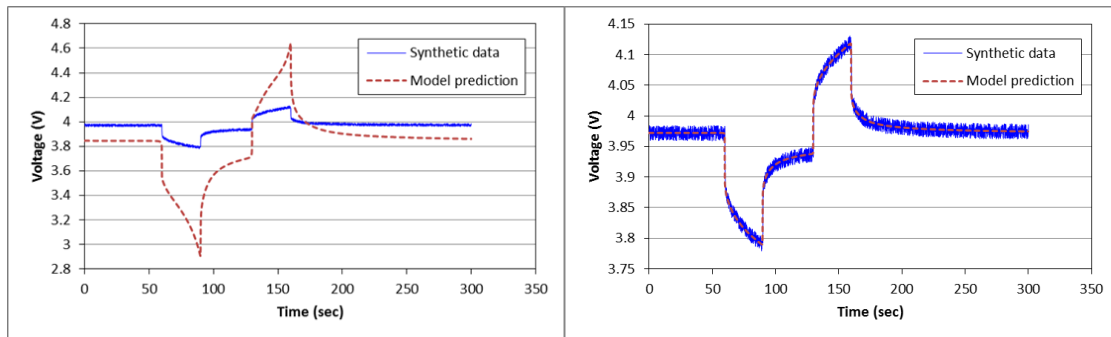
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Model vs data before (left) and after (right) at 30% SOC



Model vs data before (left) and after (right) at 40% SOC



Model vs data before (left) and after (right) at 50% SOC

Figure 12. Fitting results of reformulated pseudo-2D model to synthetic HPPC data

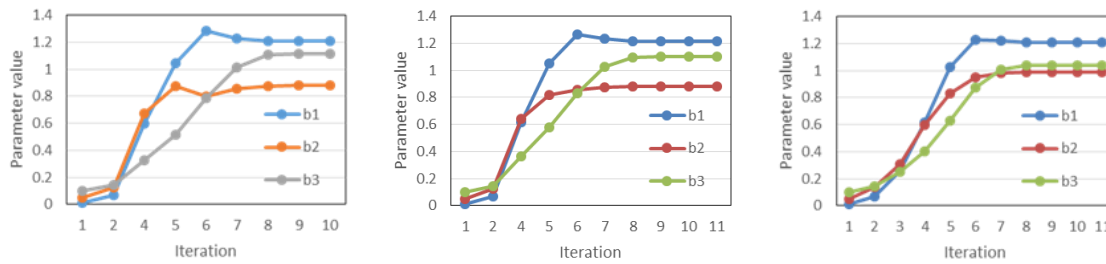


Figure 13. Convergence plots for parameters at 30% (left), 40% (center), and 50% (right) SOC

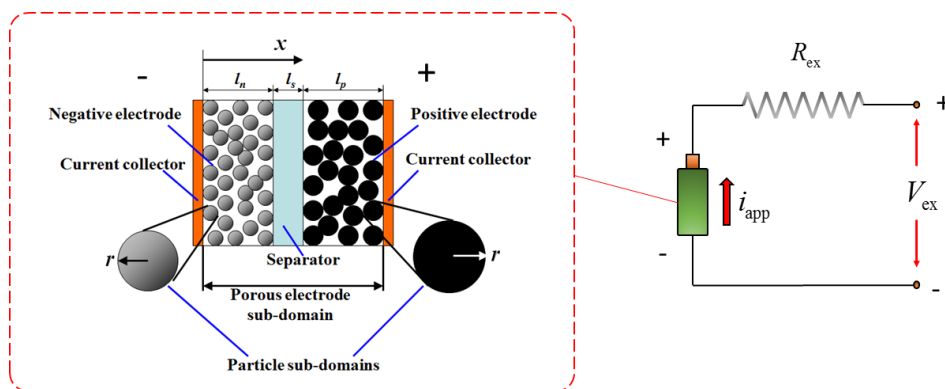


Figure 14. Illustration for Li-ion cell sandwich

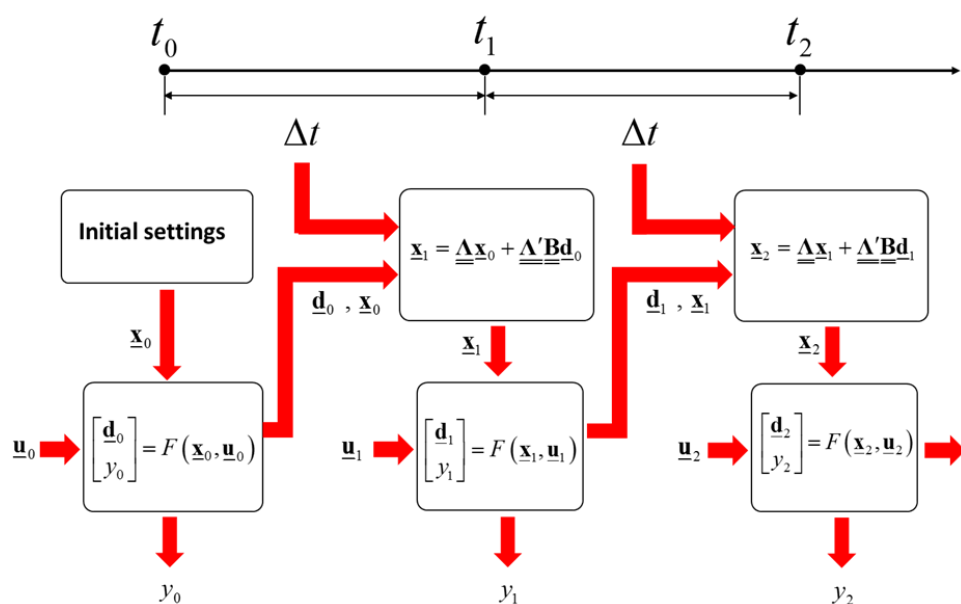


Figure 15. Illustration for the NSVM solution procedure

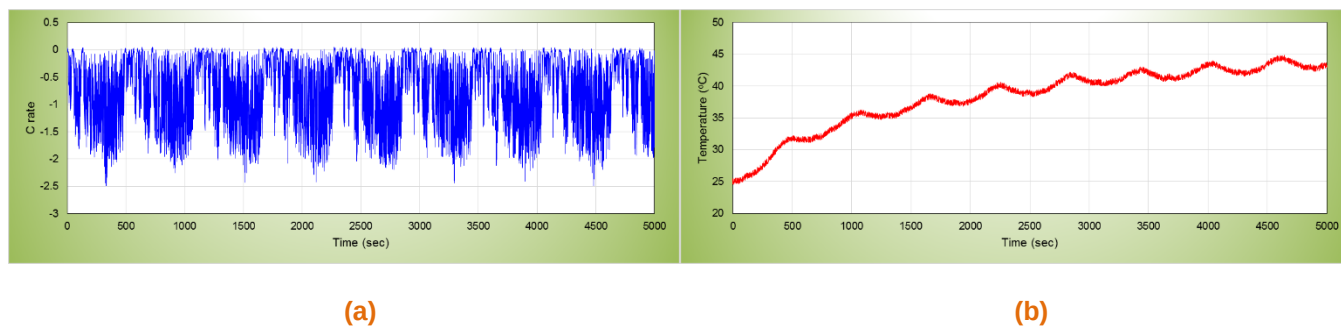


Figure 16. Synthesized current and temperature profiles for practical drive cycles:
(a) current profile, (b) temperature profile

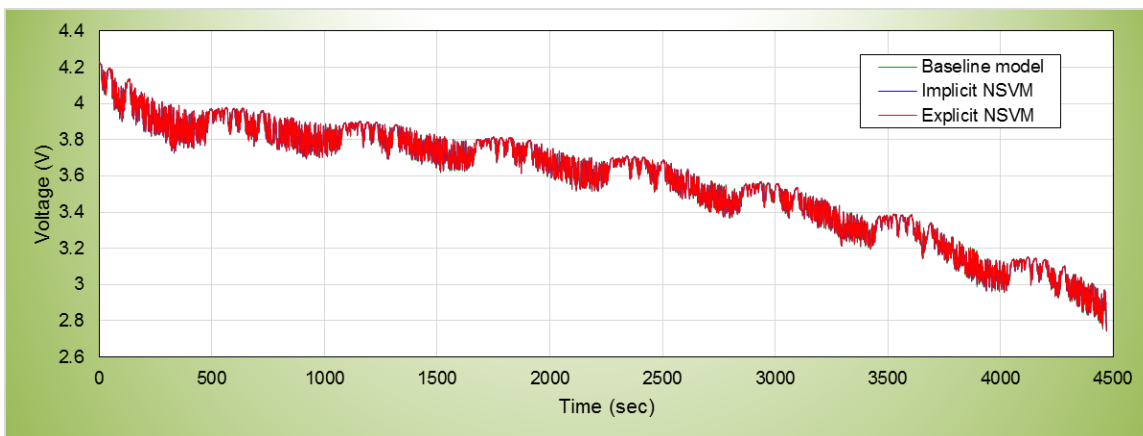


Figure 17. Simulated voltage response during drive cycle

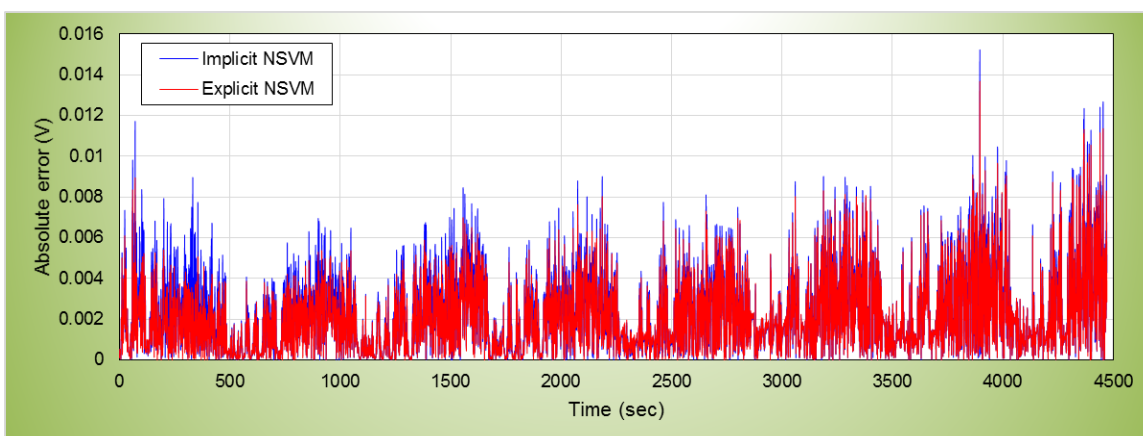


Figure 18. Absolute error of simulated voltage response

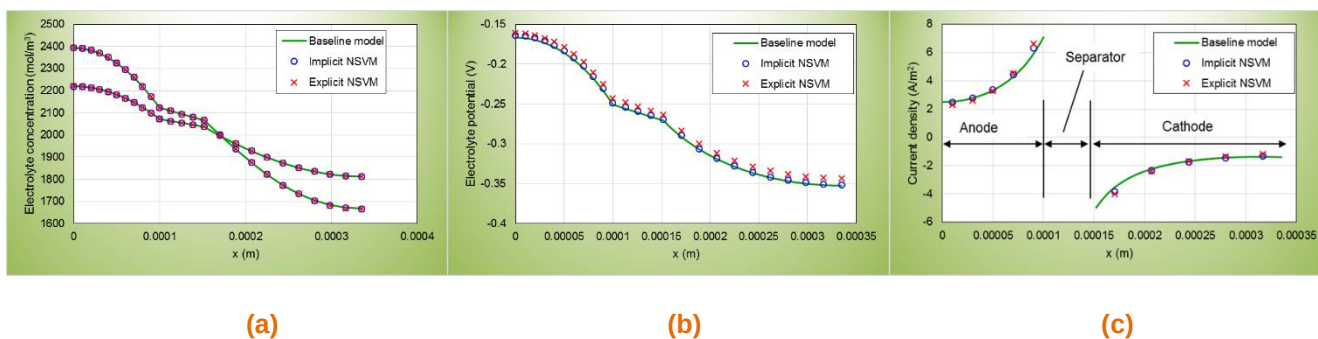
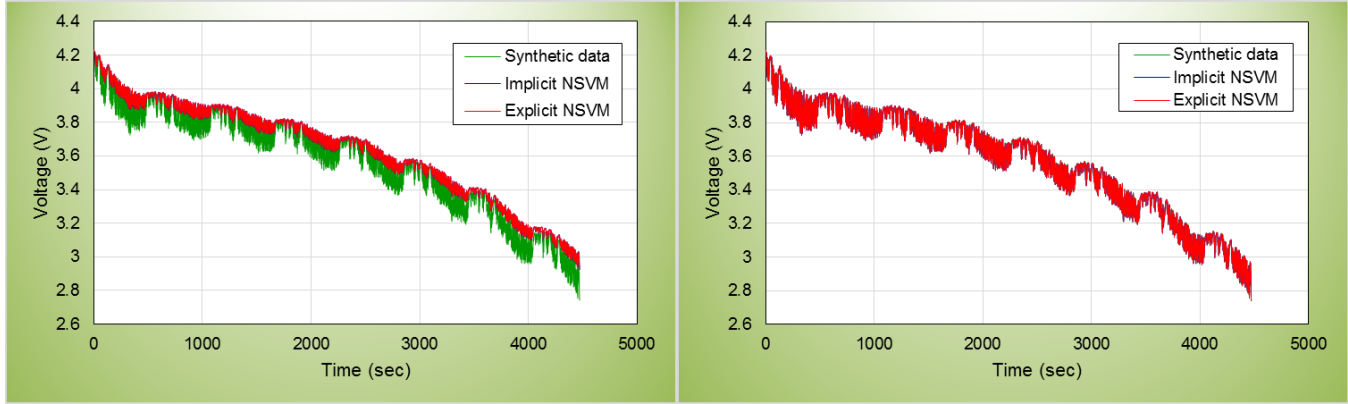


Figure 19. Simulation of distributed cell properties: (a) electrolyte concentration, (b) electrolyte potential, (c) surface reaction current density



(a)

(b)

Figure 20. Fitting NSVM to baseline model through nonlinear regression (a) NSVM vs baseline model at initial iteration (b) NSVM vs baseline model after optimization

Symbol	Value	Unit	Description
$D_{s,n}$	1.50E-14	m^2/s	Solid phase diffusion coefficient of anode
$D_{s,p}$	5.76E-14	m^2/s	Solid phase diffusion coefficient of cathode
k_n	1.00E-10	$m^{2.5}/mol^{0.5}/s$	Reaction rate constant for anode
k_p	1.00E-10	$m^{2.5}/mol^{0.5}/s$	Reaction rate constant for cathode

Table 1. Cell parameter values estimated at beginning of life

Symbol	Value	Unit	Description
U_{refs}	0.349	V	OCP for SEI reaction
i_{0s}	8.0E-04	A/m^2	Exchange current density for SEI reaction
M_{SEI}	0.108	kg/mol	Molecular mass for SEI film
ρ_{SEI}	2700	kg/m^3	Density of SEI film
K_{SEI}	3E-6	S/m	Electrical conductivity of SEI film

Table 2. Physical parameters for the SEI side reaction

Symbol	LIB4	LIB6	LIB7	Unit	Description
Ac	0.06561	0.06657	0.06633	m ²	Cross section area of electrode pair
$\epsilon_{s,p}$	0.5978	0.5919	0.5919	1	Solid phase volume fraction in cathode
$R_{f,n,0}$	0	0.016	0.016	Ohm·m ²	Film resistance for anode
$R_{f,p,0}$	0.06	0.07	0.07	Ohm·m ²	Film resistance for cathode

Table 3. Cell design parameters

Physics	Governing equations
Electrolyte mass transfer	$\epsilon_1 \frac{\partial c_1}{\partial t} + \nabla \cdot \mathbf{N}_1 = R_1 \quad \mathbf{N}_1 = -D_{l,eff} \nabla c_1 + \frac{\mathbf{i}_l t_+}{F}$ $D_{l,eff} = \epsilon_1^{1.5} D_l \quad R_1 = \frac{1}{F} \sum_k i_{v,k}$
Electrolyte charge conservation	$\mathbf{i}_s = -\sigma_{l,eff} \nabla \phi_1 + \left(\frac{2\kappa_{l,eff} RT}{F} \right) \left(1 + \frac{\partial \ln f}{\partial c_1} \right) (1 - t_+) \nabla \ln c_1$ $\nabla \cdot \mathbf{i}_l = i_{v,total} \quad \kappa_{l,eff} = \epsilon_1^{1.5} \kappa_l \quad i_{v,total} = \sum_k i_{v,k}$
Solid phase mass transfer	$\frac{\partial c_{s,k}}{\partial t} = \nabla \cdot (D_{s,k} \nabla c_{s,k})$
Solid phase charge conservation	$\nabla \cdot \mathbf{i}_s = -i_{v,total} \quad \mathbf{i}_s = -\sigma_{s,eff} \nabla \phi_s \quad \sigma_{s,eff} = \epsilon_s^{1.5} \sigma_s$
Li-ion intercalation kinetics (Butler-Volmer equations)	$i_{0,k} = F k_{r,k} (c_{s,k,max} - c_{s,k})^{\alpha_{a,k}} (c_{s,k})^{\alpha_{c,k}} \left(\frac{c_1}{c_{l,ref}} \right)^{\alpha_{a,k}}$ $i_{loc,k} = i_{0,k} \left[\exp \left(\frac{\alpha_{a,k} F \eta_k}{RT} \right) - \exp \left(-\frac{\alpha_{c,k} F \eta_k}{RT} \right) \right]$ $i_{v,k} = a_{v,k} i_{loc,k} \quad \eta_k = \phi_s - \Delta \phi_{s,k,film} - \phi_l - U_k$ $\Delta \phi_{s,k,film} = i_{total} R_{film,k}$

Table 4. List of governing equations for pseudo-2D model

	Reaction rate constants		Solid phase diffusivities	
	Anode	Cathode	Anode	Cathode
Implicit NSVM	0.857838	1.020308	1.022884	1.095047
Explicit NSVM	0.833355	1.102079	1.023376	1.103187

Table 5. The ratios for optimized parameters vs true values

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AVPTA Technology Focus Area 6: Energy Storage and Batteries

Development and Validation of a Simulation Tool to Predict the Combined Structural, Electrical, Electrochemical and Thermal Responses of Automatic Batteries

DOE-VTO TFA Lead: David Howell
TARDEC TFA Lead: Laurence Toomey

Principal Investigator:
Dr. James Marcicki

Ford Motor Company
Energy Storage Research
2101 Village Road
Dearborn, MI 48152

Project Start: Q2FY16
Estimated Completion: Q1FY19

Objective:

To develop and validate a simulation tool with unprecedented fidelity to predict the combined structural, electrical, electrochemical and thermal (SEET) response of automotive batteries to crash-induced crush and short circuit.

Strategic Context:

Lithium-ion batteries is promising for both the military and commercial vehicle applications by improving their energy efficiency and functionality through electrification. Computer aided tools will help to accelerate development and fielding safe, high-performance, and long-lasting lithium ion battery module for dual applications. The simulation tool should have unprecedented fidelity to predict the combined structural, electrical, electrochemical, and thermal (SEET) response of automotive batteries to crash-induced crush and short circuit.

Accomplishments:

- Automotive grade Li-ion cells were selected and purchased, and initial testing conducted.
- An analysis of existing models and input parameters was completed.
- Basic assumptions for the model were formulated.
- A test matrix was developed for the cells, and a test site selected.
- A preliminary version of the software has been developed and demonstrated for external short circuit and crush leading to internal short circuit scenarios.

- Techniques such as the use of layered solid elements and macro scale meshes were developed to reduce simulation complexity, and demonstrated significant reductions in calculation times.

Introduction:

This is the first year of a three-year project to develop a practical simulation tool to predict the combined structural, electrical, electrochemical, and thermal responses of automotive batteries to crash induced crush and short circuit, and validate it for conditions relevant to automotive crash. The expected benefits of the simulation tool are to reduce development time and cost by reducing the number of physical prototypes required, as well as improve the abuse response of battery systems. The project plan including major constituents and progression based on case studies is shown in Figure 1.

Approach:

- Develop innovative material constitutive models and finite element method (FEM) element formulations that capture the mechanical response of cell components, including the case material, electrodes, separator, and their interactions with electrolyte.
- Clearly identify the required input parameters for the new constitutive models, FEM element formulations, and exothermic, electrochemical reaction state equations governing multi-physics phenomena during crush-induced electrical short, thermal ramp, and overcharge conditions.
- Design and execute a test matrix encompassing automotive crash strain rates, at a number of kinetic energy levels and physical orientations likely to occur in vehicle impacts.
- Develop integrated modeling tools which demonstrate high-fidelity predictions of the onset of thermal runaway from the experimental test matrix using commercially available cells, module, and packs, spanning multiple chemistries relevant to automotive applications.
- Maintain high-fidelity predictions while exploring methods to reduce the computational complexity of the model, and deliver a practical tool that is integrated with the laboratory's Open Architecture Software (OAS), for a broad customer base within automotive product development.

Results and Discussion:

During the first three quarters of the first year, Types D & E cell hardware were selected and purchased, and initial testing begun. A test matrix was established and a test site selected.

Tensile and compressive testing of cell components is roughly 80% complete. In general, the Type D separator response is isotropic within the bounds of experimental repeatability, while the Type E separator exhibits a strong orientation dependence. Both cell types exhibit a 10 – 15% decrease in failure strain going from 0.01/s to 0.1/s strain rates, but otherwise qualitatively similar responses. The data is summarized in Figure 2.

The electrode data show a relatively brittle response, which indicates the interaction between the coating and metal current collector produces a strain localization effect.

Analyses of existing models and formulations of assumptions helped direct further development of the model. Battery multiphysics models have been developed within the LS-DYNA thermal and electromagnetism solvers. The battery model relies upon a spatially distributed equivalent circuit model that is implemented as illustrated in Figure 3.

The input parameters are dependent on state of charge and temperature, and coupling mechanisms are in place between the electrical, thermal, and structural solvers. Preliminary models were demonstrated using newly developed contact detection algorithms for a conducting metal rod contacting cell tabs to initiate an external short circuit. The simulation first uses explicit time integration, then freezes the structural response and performs implicit time integration. The setup and thermal fringe plots are summarized in Figure 4. Additional work is planned to better understand and model contact resistance.

The use of layered elements and macro-scale meshes was shown to significantly reduce computational requirements, and further development in these areas is underway. These will be key developments for the team in Budget Period 2.

Conclusions:

The first year has been successful and the project is on track. A test matrix was developed for the cells, and a test site selected. A preliminary version of the software has been developed and demonstrated for external short circuit and crush leading to internal short circuit scenarios. Techniques such as the use of layered solid elements and macro scale meshes were developed to reduce simulation complexity, and demonstrated significant reductions in calculation times.

The second year will focus on the following tasks:

- Create multi-physics framework and enhanced material models;
- Identify and obtain required model inputs;
- Integrate solvers into Alpha version model;
- Formulate development assumptions for the Beta version model;
- Select and build hardware for use in Beta model validation; and
- Create multi-physics solvers and material models for Beta model.

References:

None

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Figures:

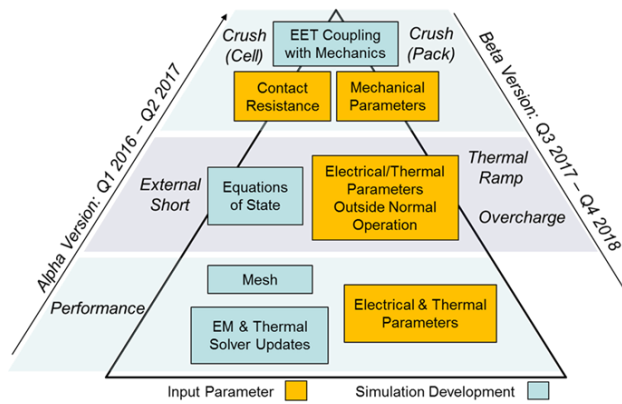


Figure 1. Project schematic showing major constituents and progression of Alpha and Beta versions.

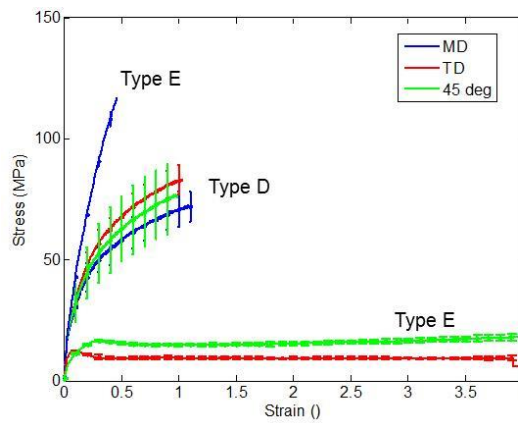


Figure 2. Separator tensile test data for two cell types, showing orientation dependence and stress-strain behavior.

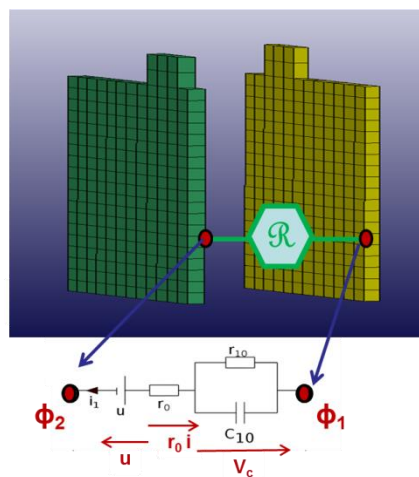


Figure 3. Separator tensile test data for two cell types, showing orientation dependence and stress-strain behavior.

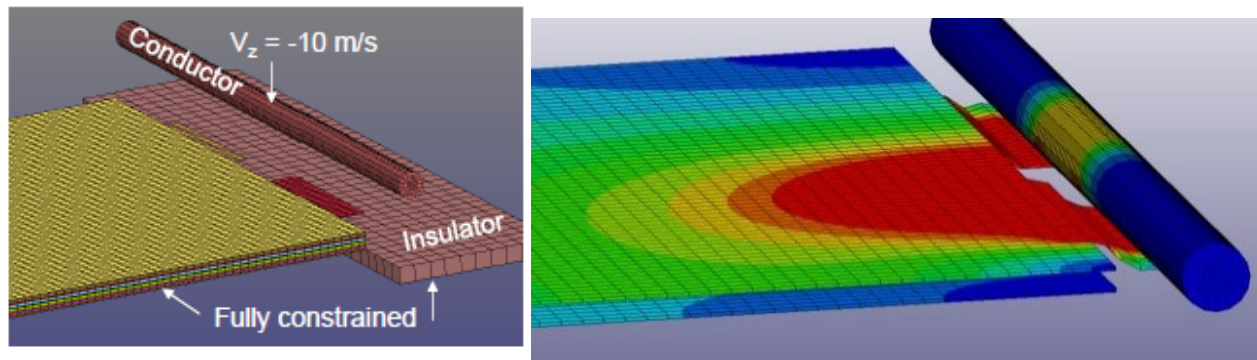


Figure 4. Model setup for a mechanically-induced external short circuit, and thermal fringe response after contact is initiated (red is warmer, blue is colder).

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AVPTA Technology Focus Area 6: Energy Storage and Batteries

Multiphysics Computer-Aided-Engineering Tools for Performance, Life, and

DOE-VTO TFA Lead: David Howell
TARDEC TFA Lead: Laurence Toomey

Principal Investigator(s):
Dr. Kandler Smith

Affiliation:
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Project Start: Q3FY16
Estimated Completion: Q4FY18

Objective:

Construct an integrated multi-physics simulation environment/tool for analysis of performance, safety and life of li-ion battery module used in military vehicles.

Strategic Context:

The energy efficiency and functionality of military vehicles through electrification can be improved with energy storage system utilizing lithium-ion battery technologies. CAE tools are capable of accelerating development fielding safe, high-performance, and long-lasting lithium ion battery module for military vehicle applications. NREL will develop a robust and efficient analysis tool for TARDEC by customizing NREL's in-house modeling tools and leveraging new functionalities being produced by continuing CAEBAT projects.

Accomplishments:

- Provided an on-site training workshop.
- Identified and reported modeling tool structures (first deliverable).
- Evaluated parallel computing in current ANSYS Fluent battery module.

Introduction:

Energy storage system based on lithium-ion batteries is promising to improve the energy efficiency and functionality of military vehicles through electrification. Computer-Aided-Engineering (CAE) tools are able to accelerate development fielding safe, high-performance, and long-lasting lithium ion battery module for military vehicle applications.

As CAEBAT[1] program performer, NREL supports DOE to develop numerical design tools to shorten design cycles and optimizing batteries for improved performance, safety, long

life, and low cost. NREL has played a leading role in numerical analysis of multiphysics behaviors of lithium-ion batteries. NREL's multi-scale multi-domain (MSMD) model overcomes the modeling challenges posed by the highly nonlinear multi-scale response of battery systems. The expandable, modular, and flexible architecture connects the physics of battery charge/discharge processes, thermal control, safety, and reliability in a computationally efficient manner.

The MSMD acts as the framework for this suite of tools being developed in this project. Performance-, life- and safety-component models will be customized and integrated as a user defined library in ANSYS Fluent, a computational fluid dynamics code in which MSMD model framework has been standardized. The user will be able to perform battery performance, life, safety and interactions analysis in a single integrated battery simulation platform. The user will further leverage enhanced capabilities being implemented in the ANSYS Fluent Battery Module as outcomes of other continued CAEBAT projects.

Approach:

The proposed CAE tool will be developed by customizing NREL's in-house modeling tools and leveraging new functionalities being produced by continuing CAEBAT projects. NREL's existing performance, life and safety model will be refined and integrated as a user defined library in ANSYS Fluent Battery Module [2], in which NREL's MSMD battery modeling framework [3] already becomes standard as a result of previous CAEBAT projects. The functionalities of the CAE tool will be verified utilizing the 6T battery form factor.

Results and Discussion:

The existing capabilities of NREL's battery performance, life and safety models were summarized and reported along with the development plan. These three component models are planned to be integrated as a user defined library in ANSYS Fluent so that related battery analysis can be performed in a single integrated battery simulation platform. One of the key challenges for model integration is the difference of temporal scales of life, performance and safety simulations. NREL is currently proposing an indirect coupling structure, as shown in Figure 1. There is no connection between the life and safety sub-models as their impact on each other is negligible.

The tool is aimed to support high performance parallel computing and simulation. NREL is evaluating the HPC performance of the ANSYS Fluent battery module. Figure 2 shows the comparison of simulation results utilizing four processors on a desktop computer and NREL's HPC system, Peregrine. The simulation condition is a 3S1P battery module under 4C constant-current discharge. With the NTGK model implemented in Fluent battery module, an empirical electrode-domain model, identical results were obtained by the PC and HPC.

As part of the knowledge transfer activities, NREL held an on-site training workshop for TARDEC at the end of August, 2016. This workshop was planned to let TARDEC users get familiar with the battery modeling platform (shown in Figure 3), current NREL modeling approaches and capabilities, and identify gaps that will be addressed under this project.

Conclusions:

The development plan has been made to construct the proposed integrated multiphysics simulation tool for analysis of performance, safety and life of li-ion battery modules. Existing capability and capability being developed is summarized and reported. The tool structure is created considering the coupling among these sub-models and challenges due to the large difference of time-scale.

References:

1. Computer-Aided Engineering for Electric-Drive Vehicle Batteries (CAEBAT). (2016). Retrieved from <http://www.nrel.gov/transportation/energystorage/caebat.html>
2. ANSYS Fluent Battery Module, Release 17.0, ANSYS Fluent Advanced Add-On Modules, ANSYS, Inc.
3. G-H. Kim, K. Smith, K-J. Lee, S.Santhanagopalan, A. Pesaran, "Multi-Domain Modeling of Lithium-Ion Batteries Encompassing Multi-Physics in Varied Length Scales," J. Electrochem Soc, Volume 158, Issue 8, pp. A955-A969 (2011)

Figures:

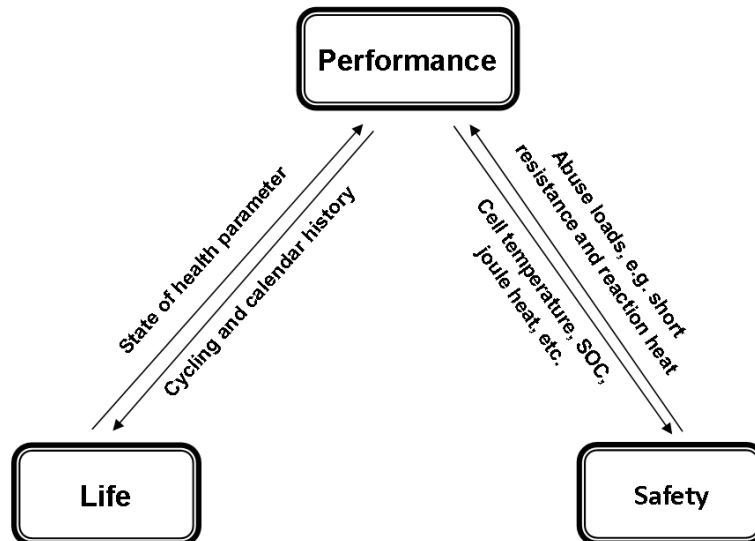


Figure 1 Indirect coupling between performance, life and safety

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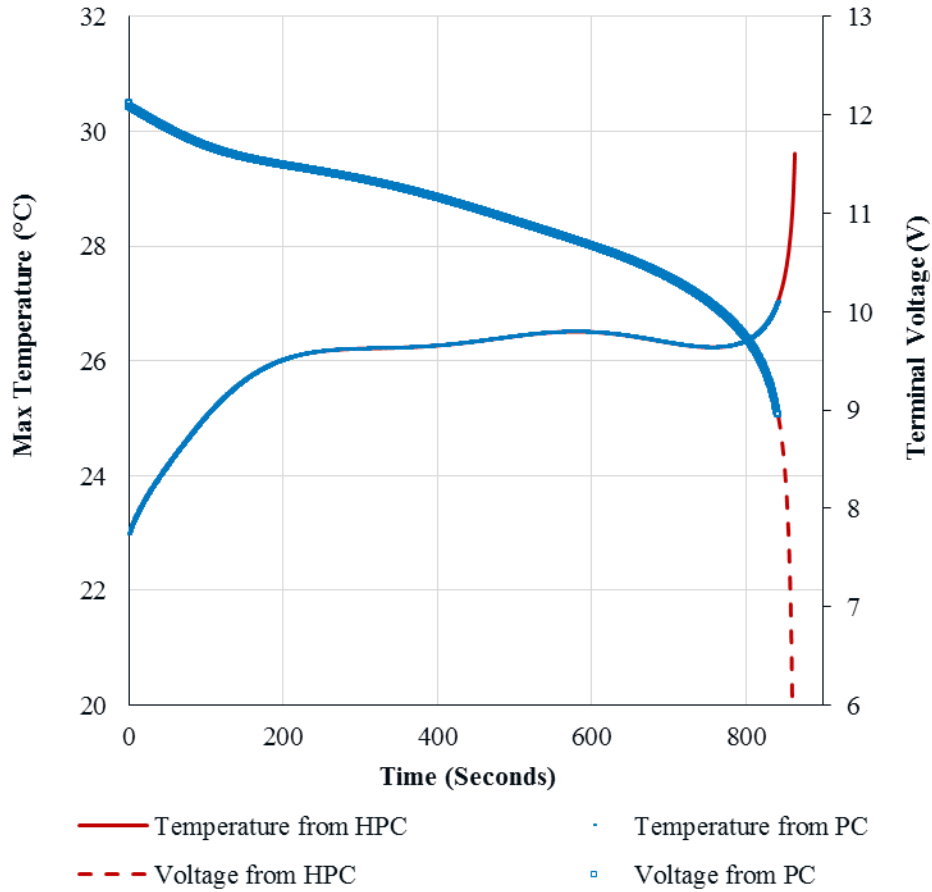


Figure 2. Comparison of simulation results of a 3S1P battery module under 4C constant-current discharge using PC and HPC

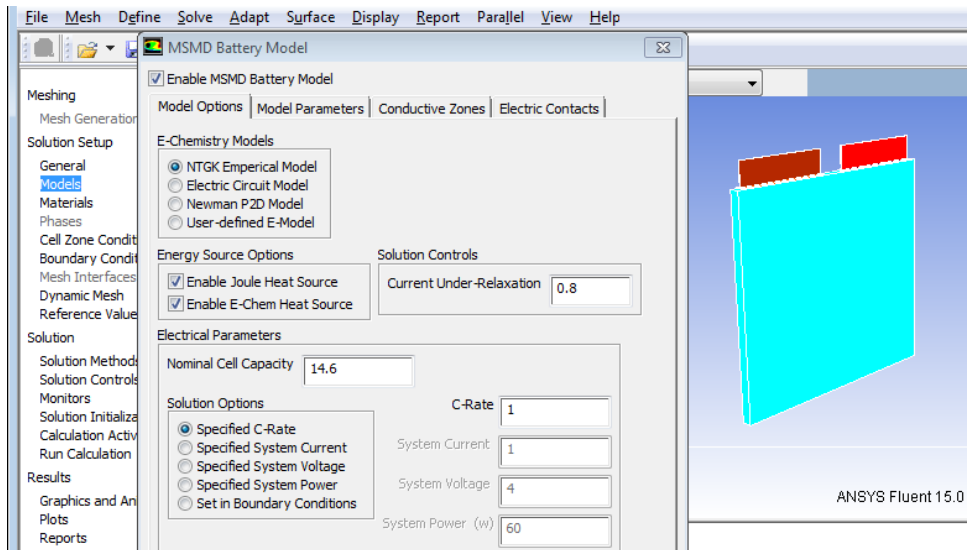


Figure 3. Graphical user interface of the MSMD battery model in ANSYS Fluent battery add-on module

AVPTA Technology Focus Area 7: Analytical Tools (Modeling & Simulation)

Physics-Based Computational Fluid Dynamics (CFD) sub-model Development

DOE-VTO TFA Lead: Leo Breton
TARDEC TFA Lead: Dr. Vamshi Korivi

Principal Investigator(s):

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Dr. Sage Kokjohn,
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Dr. Seung Hyun Kim,
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University of Wisconsin Madison,
Michigan Technological University,
Ohio State University,
Penn State University,
University of Illinois at Urbana-Champaign

Project Start: Q2FY16
Estimated Completion: Q1FY19

Objectives:

Development and validation of more accurate, physics-based mathematical sub models (fuel injection spray, cavitation within fuel injectors, flash boiling, spray/wall interaction, super critical fuel injection, in-cylinder radiation and heat transfer, engine knock and soot emissions) for use in Computational Fluid Dynamics (CFD) software.

Strategic Context:

The impact of transient mixing and charge formation during the initial stages of the fuel injection event for high pressure JP-8 injection is a research gap identified by office of Chief Scientist.

Improvement of these sub models will help develop the fire protection competency of advanced modeling and simulation tools to address emerging threats and technologies due to fuel fires inside the ground combat vehicles.

Accomplishments:

Development and validation of more accurate, physics-based mathematical sub models for use in Computational Fluid Dynamics (CFD) software have been initiated with different universities and a national lab partner for developing following eight sub models. Computational and experimental studies have been initiated for development of these sub models.

- Super critical fuel injection (Univ. of Alabama & Argonne National Labs)
- Cavitation within fuel injectors (Boston Univ & Oakridge National Labs)
- Fuel injection spray (Georgia Tech & Argonne National Labs)
- Soot emissions (Univ of Wisconsin Madison & Sandia National Labs)
- Spray/wall interaction (Michigan technological Univ & Argonne National Labs)
- Engine knock (Ohio State Univ & Oak Ridge National Labs)
- In-cylinder radiation and heat transfer (Penn State University & Oakridge National Labs)
- Flash boiling (Univ. of Illinois at Urbana-Champaign & Argonne National Labs)

Introduction:

Computational Fluid Dynamics (CFD) Software has led to improved engine designs but not yet realized full potential for attaining the goals of shortened engine development time, reducing fuel consumption, and minimizing exhaust emissions due to predictive accuracies of the sub models used in commercial and government sponsored software.

Also, it is a general consensus among academic, national Labs and industry community that there is lack of experimental data for validation of the new or improved sub-models. Developing accurate sub-models that are physics-based, predictive in nature and validated with experimental data, will require less calibration and tuning than currently available sub-models.

Approach:

Experimental protocols and apparatuses to identify the inaccuracies and formulate a technical approach to overcome.

Publication and Dissemination of information regarding improved sub models for inclusion in all commercial and government sponsored CFD codes.

Results and Discussion:

Summary of each sub model is summarized in following sections separately.

Development and Validation of Physics-Based Sub-Models of High Pressure Supercritical Fuel Injection at Diesel Conditions (Figure 1):

Developed and applied high-speed Rainbow Schlieren technique (RSD) for measurements in flames and supersonic microjets to optimize the RSD optical setup for the injector study.

Evaluated various existing equations of state and methodologies to assess their appropriateness and accuracy in describing correlations between the thermal properties and their corresponding transport properties at the high-pressure conditions.

Development & Multiscale Validation of Euler-Lagrange based Computational Methods for Modeling Cavitation within Fuel Injectors (Figure 2):

Completing validation of bubble behavior using Smoothed Particle Hydrodynamics (SPH) approach. Incorporating bubble sub-models into nozzle flows to predict bubble cavitation behavior.

Established working experimental apparatus to induce hydrodynamic cavitation in various nozzle geometry. Demonstrated two viable technique in studying cavitation dynamics.

Development and Validation of Turbulent Liquid Spray Atomization Sub-model for Diesel Engine Simulations. (Figure 3):

Kelvin-Helmholtz and Huh-Gosman spray models are implemented into OpenFoam CFD software to understand turbulence-aerodynamic interactions on spray breakup.

Spray measurements using visible laser liquid scattering extinction are completed at away from the nozzle and X-Ray Radiography (XRR) measurements are done near the nozzle.

Development and Validation of a Lagrangian Soot Model Considering Detailed Gas Phase Kinetics and Surface Chemistry (Figure 4):

A polycyclic aromatic hydrocarbons (PAH) mechanism was defined and implemented into a multi-fuel chemical kinetics mechanism to simulate gasoline, ethanol, and diesel fueled combustion.

The combined reaction mechanism shows good agreement with ignition delays from shock tubes, species profiles from burner stabilized premixed flames, and cylinder pressure and heat release from both conventional, high temperature combustion, and advanced low temperature combustion modes.

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Evaporation Sub-Model Development for Volume of Fluid (eVOF) Method Applicable to Spray-Wall Interaction Including Film Characteristics with Validation at High Pressure Temperature Conditions (Figure 5):

Complete design and fabrication of heated metal impinging plate, metal injector window, transparent impinging plate, and injector nozzle. Perform preliminary spray-wall interaction test and data analysis of key parameters. Develop optical diagnostics of Mie and schlieren for individual and simultaneous measurement.

Validation of Lagrangian-Eulerian Spray Model by means of CFD simulations of Engine combustion network Spray-A conditions consistent with nominal initial and boundary conditions of future MTU experiments.

Development of a Physics-Based Combustion Model for Engine Knock Prediction (Figure 6):

Development of the base modeling framework with the computational code. Direct Numerical Simulation (DNS) of end-gas ignition and Knock model development: Validation with DNS. Established DNS configuration and simulation approach. Performed initial DNS and analyzed premixed flame DNS data. Acquired custom hardware and capabilities that will be used for in-cylinder sampling of gas species.

Development and Validation of Predictive Models for In-Cylinder Radiation and Wall Heat Transfer (Figure 7):

Multiple Reynolds Averaged Navier-Stokes -based turbulent boundary layer wall heat transfer models have been implemented in OpenFOAM CFD software.

Initial imaging for optical access engine was done using a demo camera, awaiting delivery of the desired Infra-red camera.

Model Development for Multi-Component Fuel Vaporization and Flash Boiling (Figure 8):

Successfully demonstration of capabilities in simulating multi-component fuel vaporization for hollow cone sprays. An education course was developed and executed at the University of Illinois at Urbana Champaign, where a small group of mechanical engineering undergraduate students were recruited to design, build, and assemble the droplet generator and the experimental chamber.

Argonne National Laboratory developed the flash boiling sub-model, HRM, validated it under non-flashing condition, and performed preliminary tests of flashing boiling with different fuel types. Good progress has been made on the design and construction of the experimental chambers sub-systems and injection strategies (hollow cone injector and droplet generator).

Conclusions:

Both Computational and experimental efforts are underway for developing eight different sub-models. Four project leads are using open source software for development and four universities are working with a commercial software vendor to implement these sub models.

After FY17 quarter I, Go or No-Go decisions will be made for budget period II.

References:

None

Figures and Tables:

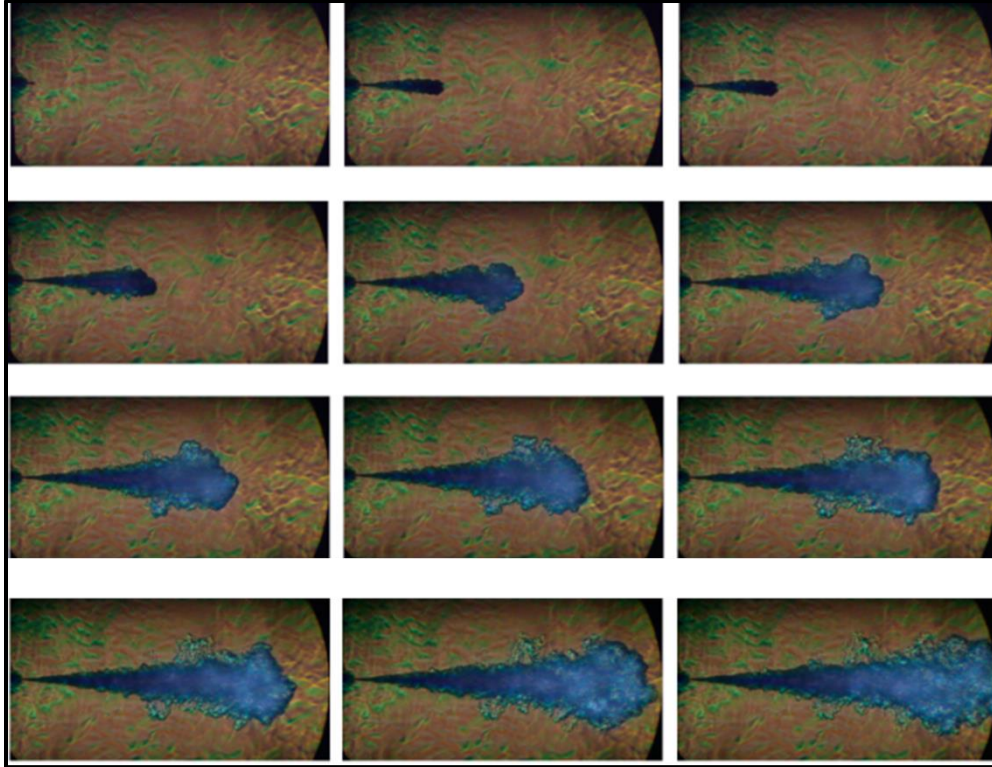


Figure 1. Rainbow Schlieren (RSD) images during fuel injection.

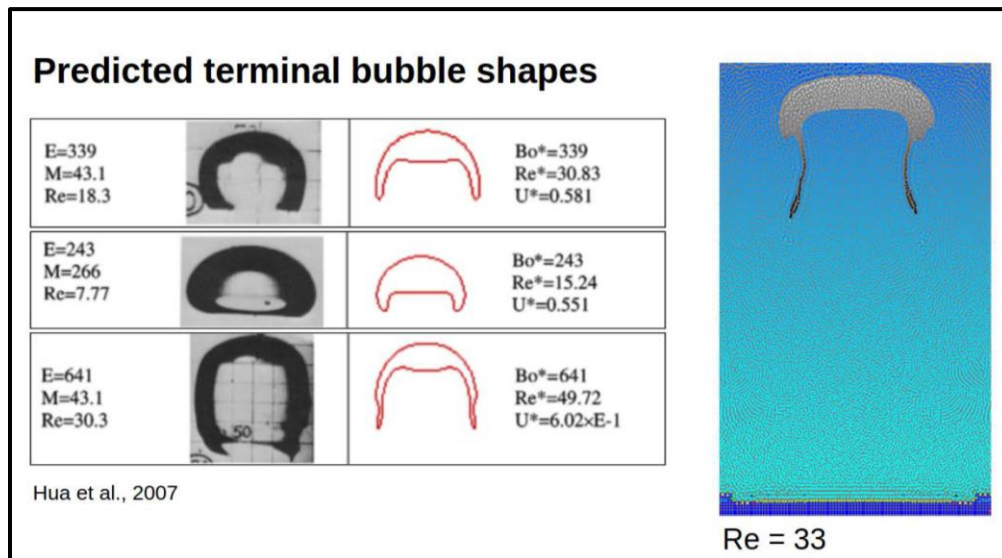


Figure 2. Experimental Data from [Hua et al 2007] (left);
Initial SPH Simulation of a Bubble in a Hydrostatic Tank

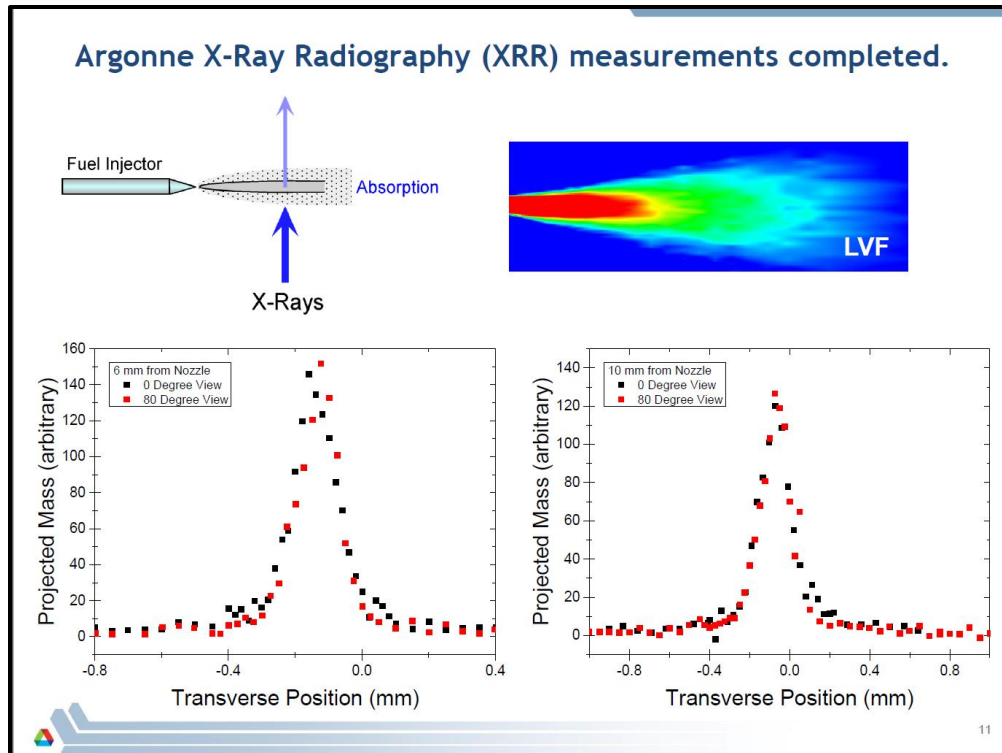


Figure 3. Turbulent Liquid Spray Atomization

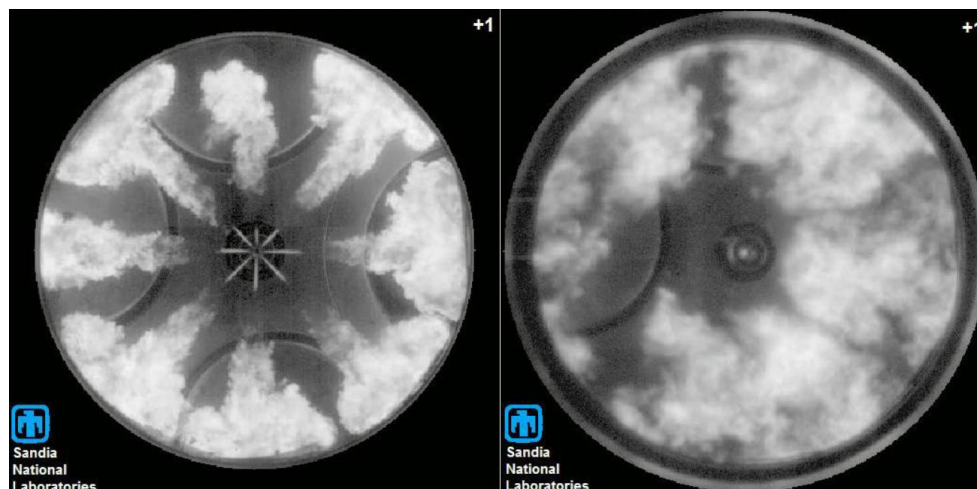


Figure 4. High Speed Imaging Demonstration of Conventional Diesel Combustion (left) and Low Temperature Combustion (right)

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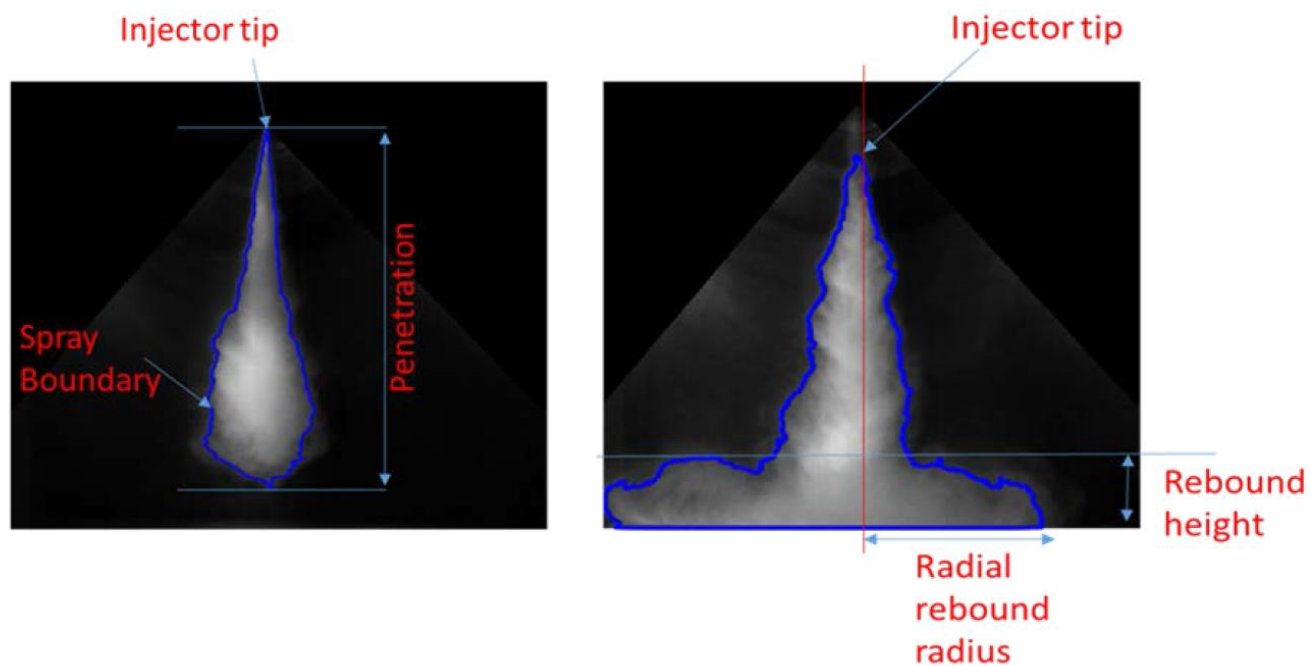


Figure 5. Imaging Process for Spray Wall Test

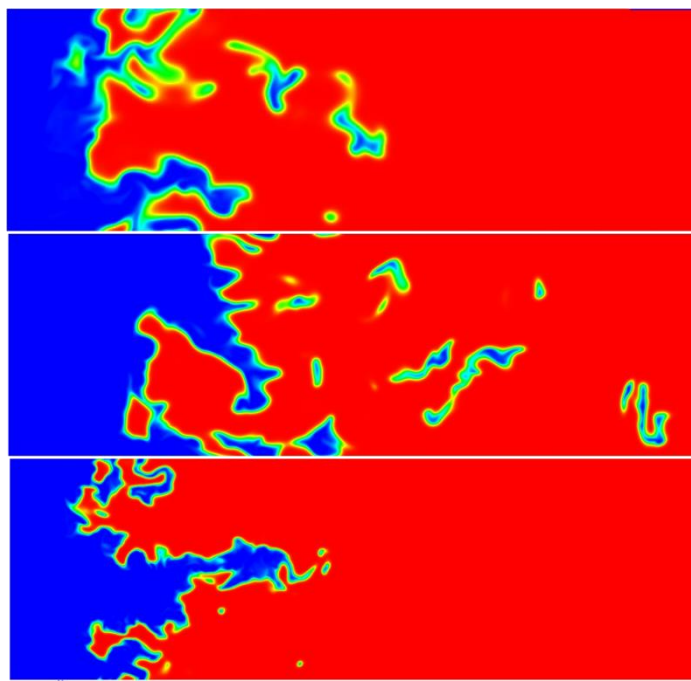


Figure 6. Progress variable (normalized temperature) field in single-step chemistry Direct Numerical Simulation

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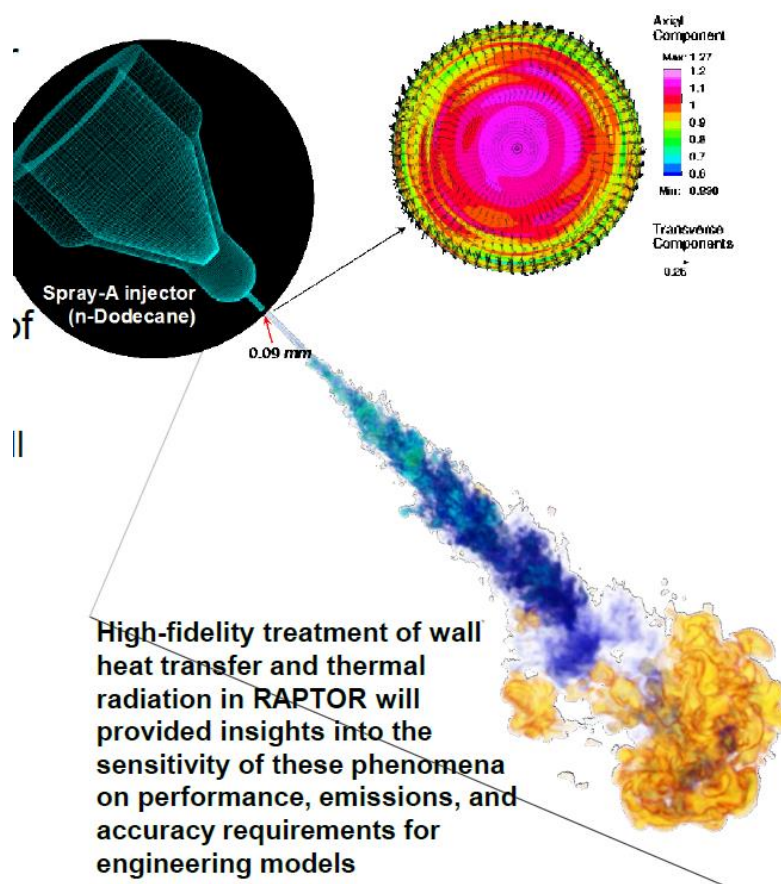


Figure 7. High-fidelity treatment of wall heat transfer and thermal radiation

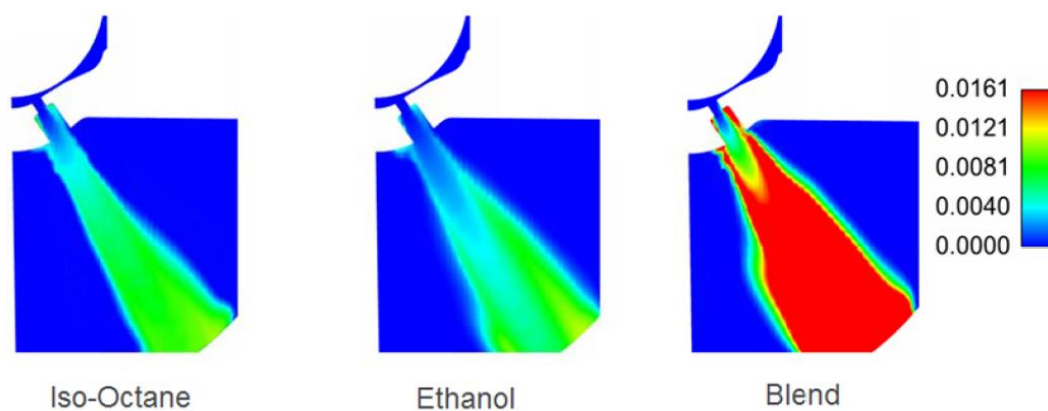


Figure 8. Predicted Vapor Mass Fractions using Computational Fluid Dynamics

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AVPTA Technology Focus Area 9: Autonomy-enabled Technologies

DOE-VTO TFA Lead: David Anderson
TARDEC TFA Lead: Dr. Rob Karlsen

There was no project activity under this TFA during FY16.

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APPENDIX A

Memorandum of Understanding

Between

U. S. Department of Energy

And

U. S. Department of Defense

Concerning Cooperation in a Strategic Partnership to Enhance Energy Security

I. Purpose

The purpose of this Memorandum of Understanding (MOU) is to identify a framework for cooperation and partnership between the Department of Energy (DOE) and the Department of Defense (DOD), hereafter referred to as the Parties, to strengthen coordination of efforts to enhance national energy security, and demonstrate Federal Government leadership in transitioning America to a low carbon economy. This MOU covers, but is not limited to, efforts in the areas of energy efficiency, renewable energy, water efficiency, fossil fuels, alternative fuels, efficient transportation technologies and fueling infrastructure, grid security, smart grid, storage, waste-to-energy, basic science research, mobile/deployable power, small modular reactor nuclear energy, and related areas.

II. Legal Authority

DOE enters into this MOU under the authority of section 646 of the Department of Energy Organization Act (Pub. L. 95-91, as amended; 42 U.S.C. § 7256). DOD enters into this MOU under the authority of DOD Instruction 4000.19 "Inter-Service and Intra-Governmental Support" August 9, 1995.

III. Background

In the 2010 Quadrennial Defense Review, the DOD expressed an intent to partner with other U.S. agencies to research, develop, test, and evaluate new sustainable energy technologies. The DOD aims to speed innovative energy and conservation technologies from laboratories to military end users, and it uses military installations as a test bed to demonstrate and create a market for innovative energy efficiency and renewable energy technologies coming out of DOE laboratories, among other sources. The DOE is currently supporting a range of projects aimed at improving energy efficiency and renewable energy efforts across the military services.

Energy security for the DOD means having assured access to reliable supplies of energy and the ability to protect and deliver sufficient energy to meet operational and Installation energy needs. Energy efficiency can serve as a force multiplier, increasing the range and endurance of forces in the field while reducing the number of combat forces diverted to protect energy supply lines, as well as reducing long-term energy costs. DOD is also increasing its use of renewable energy supplies and reducing energy demand to improve energy security and operational effectiveness, reduce greenhouse gas (GHG) emissions in support of U.S. climate change initiatives, and protect the DOD from energy price fluctuations. Solving military challenges through innovation has the potential to yield spin-off technologies that benefit the civilian community as well.

The DOE is the lead Federal agency responsible for the development and deployment of advanced energy technologies, yet DOD will need to invest in many of these same energy technologies as well as other energy technologies which may be unique to DOD's operational requirements. Partnering with DOD provides DOE the opportunity to accelerate the deployment of its technologies and expertise toward the critical economic and energy security needs of the United States and to promote scientific and technological innovation.

The Parties acknowledge the significant positive collaboration that already exists between DOE and DOD and intend through this MOU to strengthen and broaden that cooperation.

IV. Activities

Specific activities covered under this MOU include, but are not limited to:

- A. Evaluate energy systems and technology management solutions that meet DOD objectives including developing energy technologies that meet DOD energy requirements. Work collaboratively to identify a strategy for their development and deployment.
- B. Maximize DOD access to DOE technical expertise and assistance through cooperation in the deployment and pilot testing of emerging energy technologies. Technology areas may include, but are not limited to, energy efficiency, renewable energy, water efficiency, fossil fuels, alternative fuels, efficient transportation technologies and fueling infrastructure, grid security (e.g., superconductivity, power, electronics, microgrids, cyber, EMP), smart grid, storage, waste-to-energy, basic science research, mobile/deployable power, small modular reactor nuclear energy, and related areas.

- C. Expand cooperation related to energy management practices and knowledge exchange, working to ensure that Federal leadership is in compliance with all statutory and Executive Order goals and objectives, particularly in the area of GHG reductions. Encourage the sharing of data, including, but not limited to, data on internal energy management projects and technical assistance projects.
- D. Collaborate on science and technology (S&T) projects at research institutions sponsored by either agency. Synchronize research and development (R&D) of new knowledge and technologies to expand complementary efforts.
- E. Develop joint initiatives for major energy technology research, development and demonstration programs of mutual interest to DOD and DOE, such as pilot or demonstration facilities which address military needs and also may address national security needs that transcend military requirements. DOD installations may serve as test beds for such technical demonstrations.
- F. Develop human capital within DOE and DOD through teaching and education. Work to integrate respective agency energy training and knowledge exchange practices.
- G. Encourage professional exchanges and formal liaison relationships between all DOE and DOD components including, but not limited to, laboratory, headquarters, military installations, combatant command headquarters, and forward operating bases.
- H. Collaborate on issues regarding nuclear power, except naval nuclear propulsion, including developing a business, licensing and regulatory strategy as appropriate, and evaluating the integration of energy technologies with other industrial applications that support DOD objectives for energy security and GHG reduction. Collaboration will include NRC review and licensing of nuclear power plants that are deployed for DOD purposes, and are located on or adjacent to DOD U.S. installations.

V. Implementation

DOE and DOD intend to develop and conduct cooperative activities relating to identified high priority energy strategic needs, where such cooperation contributes to the efficiency, productivity, and overall success of the activity. The Parties intend for the activities to be executed under the MOU to be established by a joint DOE/DOD senior-level Executive Committee. This Executive Committee will be co-chaired by a designee of the Under Secretary of Defense (Acquisition,

Logistics and Technology) and a designee of the Deputy Secretary from DOE. The Executive Committee will be responsible for the operations and governance of this MOU. Under the direction of the Co-Chairs, the Committee will include representatives from each of the principal DOE offices, specifically, the Office of the Under Secretary for Science, the National Nuclear Security Administration, and the Office of the Under Secretary for Energy. From the Department of Defense representatives will include the Deputy Under Secretary of Defense (Installations and Environment) and the Director of Operational Energy Plans and Programs. Additional members from both Agencies that may be involved in issues or functions of this MOU may be added. Upon agreement of both Departments, the Co-Chairs will appoint a team to develop, within 60 days, a charter and operating structure, membership, products, and decision processes.

The Executive Committee may establish working groups of Federal employees to perform and execute necessary activities contemplated by this MOU at their discretion. The Executive Committee and its working groups may make consensus recommendations based on their collaboration.

The Executive Committee will determine an appropriate regular meeting schedule, not to be less than four times annually. The Co-Chairs will be responsible for the development and distribution of agendas, presentations, and minutes of each meeting. Action items will be clearly identified and tracked in the minutes.

The Co-Chairs will be responsible for any reporting to the appropriate Departmental Secretarial Officers and will outline accomplishments, issues, redirections, and change assessments. The reporting will be coordinated by the Co-Chairs as appropriate.

The Co-Chairs will be responsible for any reports or presentations that are requested by other organizations, subject to the necessary review of each Party.

VI. Funding

Each party intends to coordinate their individual funding and resource decisions in order to maximize the benefits of cooperation under this MOU. Any transfer of funds or sharing of resources between the parties will be pursuant to a separate or pre-existing agreement.

VII. General

Work under this MOU will be jointly planned and monitored by the DOD and DOE.

In the event any activity undertaken by the agencies to implement the purposes of this MOU involves access to and sharing or transfer of technology subject to patents or other intellectual property rights, such access and sharing or transfer will be provided on terms which recognize and are consistent with the adequate and effective protection of intellectual property rights.

This MOU is strictly for internal management purposes for each of the Parties. It is not legally enforceable and shall not be construed to create any legal obligation on the part of either Party. This MOU shall not be construed to provide a private right or cause of action for or by any person or entity.

This MOU in no way restricts either of the Parties from participating in any activity with other public or private agencies, organizations, or individuals.

This MOU is intended to complement, and not to duplicate, cooperation by the Parties under the Memorandum of Understanding between the Department of Energy (National Nuclear Security Administration)/(Office of Science)/(Office of the Under Secretary) and the Department of Defense (Acquisition, Technology and Logistics) concerning Cooperation in a Strategic Partnership to Enhance National Security of January 26, 2009.

All agreements herein are subject to, and will be carried out in compliance with, all Federal applicable laws, regulations and other legal requirements.

This MOU is neither a fiscal nor a funds obligation document. Nothing in this MOU authorizes or is intended to obligate the Parties to expend, exchange, or reimburse funds, services, or supplies, or transfer or receive anything of value.

VIII. Contacts/Designated Representatives

Under Secretary for Science
U.S. Department of Energy
Washington, DC 20585

Under Secretary for Energy
U.S. Department of Energy
Washington, DC 20585

Under Secretary for Nuclear Security
U.S. Department of Energy
Washington, DC 20585

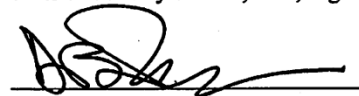
Deputy Under Secretary of Defense
Installations and Environment
U.S. Department of Defense
Washington, DC 20301

Director of Operational Energy Plans and Programs
U.S. Department of Defense
Washington, DC 20301

Deputy Assistant to the Secretary of Defense for Nuclear Matters
U.S. Department of Defense
Washington, D.C. 20301-3050

IX. Duration of Agreement

This MOU is effective on the date of the final signature and will remain in effect until it is terminated by mutual agreement of the Parties or by either Party providing ninety days written notice to the other. This MOU may be modified at any time by written agreement of the Parties. Nothing in this MOU shall be interpreted to limit or otherwise affect any authorities, powers, rights, or privileges accorded to DOD or DOE or any of the officers, employees, or organizational units under any statute, rule, regulation, contract, or agreement.



Daniel B. Poneman
Deputy Secretary of Energy

JUL 22 2010

Date



William J. Lynn III
Deputy Secretary of Defense

JUL 22 2010

Date

APPENDIX B



The Deputy Secretary of Energy
and
The Under Secretary of the Army



CHARTER

Advanced Vehicle Power Technology Alliance

I. DESIGNATION

By authority of this charter, effective on July 18, 2011, the Advanced Vehicle Power Technology Alliance (AVPTA) was established. AVPTA shall be active until the charter is rescinded, repealed, terminated, or suspended.

II. MISSION

The AVPTA is a partnership between the Department of the Army (DA) and the Department of Energy (DOE) in accordance with Section IV. E of the Department of Defense (DoD) and DOE Memorandum of Understanding (MOU) Concerning Cooperating in a Strategic Partnership to Enhance Energy Security, for the establishment of a joint technology research initiative in the area of ground vehicle power technology research, development, and transition. The seven focus areas of science and technology are: (1) advanced combustion engines and transmissions, (2) lightweight structures and materials, (3) energy recovery and thermal management, (4) alternative fuels and lubricants, (5) electrified propulsion systems, (6) energy storage & batteries, and (7) autonomy-enabled technologies. Where requirements are common, the two Departments will leverage resources to improve transition of technologies into both the commercial and military marketplace. The AVPTA leverages industrial research and development involving commercial automotive and defense ground vehicle manufacturers to transition technologies and increase precompetitive research and development.

III. RESPONSIBILITY

The AVPTA is designated as the DA's and DOE's primary point of contact for automotive power technology in the seven focus areas of science and technology. Consistent with applicable law, regulation, and policy the AVPTA may conduct its activities in accordance with such agreements as are deemed necessary for its efficient operation.

IV. AUTHORITY

The AVPTA is jointly led by the Director, U.S. Army Tank Automotive Research, Development and Engineering Center, and the Department of Energy Director, Vehicle Technologies Office (hereinafter "Directors"). Both Directors maintain authorities over their

respective budgets. The AVPTA conducts activities in accordance with the DoD-DOE Energy Security MOU. DOE entered into the MOU under the authority of section 646 of the DOE Organization Act (Pub. L. 95-91, as amended; 42 U.S.C.). The Army entered into the MOU under the authority of DoD Instruction 4000.19, "Inter-Service and Intra-Governmental Support," April 25, 2013. The Directors are the principal and primary points of contact for the prioritization of automotive/ground vehicle power and energy technologies in the seven focus areas of science and technology.

V. COORDINATION

The AVPTA shall, as appropriate, coordinate activities and actions with associated government agencies, industries, and academia with a focus on efficient vehicle power systems. The AVPTA will conduct a yearly meeting to coordinate science and technology (S&T) activities, and will align S&T projects and products where requirements are similar. A yearly meeting will be conducted to assess results, update requirements, and determine new joint efforts. The AVPTA will report results to the Under Secretary of the Army and the Deputy Secretary of Energy.

VI. ADVISORY BOARD

The Directors may establish a Senior Advisory Board with other government agencies to review strategic planning and make recommendations on future activities. All activities associated with the Senior Advisory Board will comply with the Federal Advisory Committee Act (FACA), 5 U.S.C. App. 2 and implementing regulation and policy, as applicable. As authorized by law, regulation, and policy, the Senior Advisory Board may seek the individual advice of non-Government employees (e.g., individual members of industry or academia) to secure facts and other information to assist the Senior Advisory Board's review.

VII. LEGAL AUTHORITY

The Directors will ensure that AVPTA activities are conducted in a manner consistent with all applicable laws, regulations, and policies. In particular, the appropriate agency counsel will review in advance all interaction with industry, academia, or other non-governmental entities to confirm that any necessary enabling authorities exist and to ensure compliance with the FACA and implementing regulations and policies.

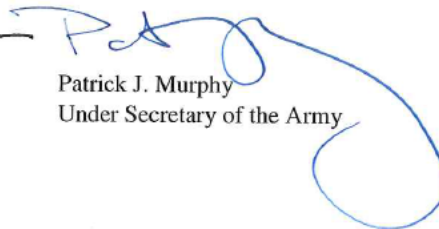
VIII. TERMINATION AND REVIEW

This charter shall terminate automatically on the 5-year anniversary date unless the undersigned expressly approves it for renewal. Directors will review this charter biannually on its anniversary date to ensure currency, completeness, and adequacy. Changes to mission

and/or responsibilities will require the review by, and approval of, the Secretary of the Army and the Secretary of Energy.



Elizabeth Sherwood-Randall
Deputy Secretary of Energy



Patrick J. Murphy
Under Secretary of the Army

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